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MACHINE CALCULATIONS OF ENERGY TRANSFER PHENOMENA IN A BOMBARDED LATTICE

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MACHINE CALCULATIONS OF ENERGY TRANSFER PHENOMENA IN A BOMBARDED LATTICE

* * * * *

Warren L. Gay

MACHINE CALCULATIONS OF ENERGY TRANSFER PHENOMENA IN A BOMBARDED LATTICE

by

Warren L. Gay
Lieutenant, United States Navy

Submitted in partial fulfillment of
the requirements for the degree of

MASTER OF SCIENCE
IN
PHYSICS

United States Naval Postgraduate School
Monterey, California

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This work is accepted as fulfilling
the thesis requirements for the degree of
MASTER OF SCIENCE
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ABSTRACT

This computer simulation investigates the ways in which an embedding lattice influences a collision event. Low energy events were studied with a Born-Mayer potential function; high energy with a Thomas-Fermi-Firsov potential. Conclusions were: (1) the lattice will increase ranges for particle energies above 400 ev; (2) the apparent mass concept is not a valid description of events in a lattice; (3) lattice effects will significantly modify the low energy portion of the target atom energy distribution function; (4) there is no evidence that a copper atom will "rebound" from a copper lattice.

The writer wishes to express his appreciation for the assistance and encouragement given him by Associate Professor Don E. Harrison, Jr. of the U. S. Naval Postgraduate School in this investigation.

TABLE OF CONTENTS

Section	Title	Page
1.	History	1
2.	Objective	6
3.	Procedure	7
4.	Potentials	12
5.	Results	13
6.	Conclusions	18
Appendix		
I	General Discussion of the Program	45
II	Block Diagram	48
III	Detailed Flow Chart	52
IV	Definition of Variables	73
V	Program Listing	78
VI	Potentials	90

LIST OF ILLUSTRATIONS

Figure		Page
1.	The Model	20
2.	Face (100) of Lattice Core	21
3.	Impact Area	22
4.	Typical Computer Output	23
5.	Typical Computer Output	24
6.	Triangular Computer Output	25
7.	Geometrical Effects of the Lattice Face	26
8.	Geometrical Effects on 100 ev Bullet	27
9.	Output Triangle for 80 ev Bullet	28
10.	Output Triangle for 40 ev Bullet	29
11.	Output Triangle for 25 ev Bullet	30
12.	Output Triangle for 100 ev Bullet	31
13.	Output Triangle for 80 ev Bullet	32
14.	Output Triangle for 40 ev Bullet	33
15.	Output Triangle for 25 ev Bullet	34
16.	Output Triangle for 100 ev Bullet	35
17.	Output Triangle for 80 ev Bullet	36
18.	Output Triangle for 40 ev Bullet	37
19.	Output Triangle for 25 ev Bullet	38
20.	Output Triangle for 5 kev Bullet	39
21.	Output Triangle for 10 kev Bullet	40
22.	Output Triangle for 30 kev Bullet	41
23.	Output Triangle for 5 kev Bullet	42
24.	Output Triangle for 10 kev Bullet	43
25.	Output Triangle for 30 kev Bullet	44

1. History.

Radiation damage is the overall term applied to erosion, disruption, or rearrangement of a crystal lattice by bombardment of ions or atoms. Sputtering, a phenomena sometimes observed in radiation damage, applies to the process of lattice atoms being ejected or "knocked out" of the crystal. The sputtering process was first observed in 1852 by Grove[1] in the cathodes of electrical discharge tubes.

Since Grove's observation, experimental and theoretical physicists have been attempting to develop a sputtering theory that will predict measurable experimental quantities as a function of mass ratio, position in the periodic table, energy of bombarding particle and angle of incidence. To date, no such complete theory is available.

A tremendous volume of material has been written on the subject of sputtering since its discovery. In 1955, Irvine[2] listed 306 papers concerned with the sputtering process. These early papers disagree violently because important experimental conditions were not obtained or simply ignored; consequently many of the conclusions reached are contradictory.

During this period two important theories were proposed. Kingdon and Langmuir[3], in 1923, developed a momentum transfer theory which agreed quite well with experimental data they had obtained for thoriated tungsten filaments. The "evaporation theory" was proposed in 1928 by von Hippel and Blechschmidt[4] and improved by Townes[5] in 1944. It assumes that the incident

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[1] W. R. Grove, Phil. Trans. Roy. Soc. London, 142, 87 (1842).

[2] M. M. Irvine, Dissertation, Lehigh University (1955).

[3] K. H. Kingdon and I. Langmuir, Phys. Rev. 22, 148 (1923).

[4] A. von Hippel and E. Blechschmidt, Ann. Physik 86, 1006 (1928).

[5] C. H. Townes, Phys. Rev. 65, 319 (1944).

particles heat a small volume of the crystal to a very high temperature and subsequently surface atoms evaporate. More recently (1953), Harrison[6], following a suggestion made by Keywell[7], presented a statistical theory of sputtering which could be placed somewhere between the two models mentioned above. We will not present details of these theories. We must mention however, that they do not provide an adequate description of the sputtering process.

The trend in sputtering theories has recently been toward the consideration of the individual collision processes within the lattice. Henschke[8] has used this approach in his theory of sputtering and Harrison and Magnuson[9] have also applied it, with modifications, to the theoretical study of sputtering threshold energies.

The theoretical work performed by Henschke uses the momentum transfer concept initiated by Kingdon and Langmuir[3] to account for all the experimental phenomena observed at low incident particle energy. His basic treatment of collisions between atoms in a lattice is based on the assumption

> ...that the collisions described can be treated with the general principles of classical mechanics, using impulsive forces, in a manner similar to the well-known collisions with restitution.[10]

However, he did not in all cases use the masses of the individual particles involved in the equations pertaining to the two body collisions. Instead he postulated an "effective" mass. If the collision is between a surface

[6] D. E. Harrison, Jr., Phys. Rev. 102, 1473 (1956).

[7] F. Keywell, Phys. Rev. 87, 160 (1952).

[8] E. B. Henschke, Phys. Rev. 106, 737 (1957).

[9] D. E. Harrison and G. D. Magnuson, Phys. Rev. 122, 1421 (1961)

[10] See reference 8, p. 738.

atom and a moving ion or atom and is such that the surface atom is struck on its "inside" hemisphere, according to Henschke, an effective mass is not required and the two particles involved can be considered to have their actual masses. Should the collision of an atom or ion be directed inward from the target lattice surface, Henschke states,

> The bulk of the target is behind the struck atom and produces a very large 'effective' mass compared to the mass of the ion or to the mass of the target atom.[11]

The reason Henschke did not assume pure elastic collisons was stated as

> Energy losses are due to the fact that the target atom is coupled rather strongly with the atoms of the lattice. Before the moment of highest compression is reached, the ion and the struck atom exchange energy with the neighboring atoms of the lattice. Debye waves are thus excited and dissipated irreversibly into the lattice.[12]

He goes on to state,

> ...the final step in each sputtering process at any angle of incidence of the ion can be generally described as a collision of the ion with an upper surface atom, in which this atom is hit on its inside hemisphere so as to obtain an impulse with a component in the direction of the outward normal to the surface. If the energy transferred in this direction to this target atom by the impact of the ion is equal to or greater than the heat of vaporization, with which the atom is assumed to be bound to the crystal lattice plane, then this atom is ejected in the collision.[13]

Early study in radiation damage was precipited by the advent of the nuclear reactor. Recently however, with the imminent possibility of thermonuclear power production and ion propulsion engines for space vehicles, other practical applications of the processes involved in radiation damage have

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[11] E. B. Henschke, Phys. Rev. 121, 1290 (1961).

[12] See reference 8, p. 738.

[13] See reference 8, p. 737.

become extremely important.

Robinson and his co-workers[14] have made theoretical studies of the ranges in solids of atoms having energies from 1 to 100 kev using digital computer techniques on the basic assumption that the moving atom loses its energy through repeated binary elastic collisions with atoms of the solid. The masses used in these calculations are the true masses of the interacting particles, but they note that their assumption is certainly not valid below 100 ev. Gibson et. al.[15] have also taken advantage of the speed available with modern digital computers in the study of radiation damage. They do not assume binary collisions but instead use iteration techniques employing Newton's equation of motion to solve the complex many body problem. The initial success of these programs have encouraged their originators to explore further the possibilities of these techniques. Although the computer programs are designed to study radiation damage, the basic principles involved are also important in sputtering.

The work just discussed is very sensitive to the mathematical form of the interatomic potential. The Born-Mayer, Bohr (screened Coulomb), and the Thomas-Fermi-Firsov are some of the potentials used in these calculations. The ability of any of the potential functions to describe a physical situation is highly dependent upon the energy range under consideration and the specific atoms or ions involved. No single potential has yet been devised that satisfactorily represents the interaction under all circumstances.

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[14] O. S. Oen, D. K. Holmes, and M. T. Robinson, Jour Appl. Phys. 34, 302 (1963).

[15] J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, Phys. Rev. 120, 1229 (1960)

An obvious unresolved question is inherent in these theories. The many body approach and the two body assumption, with a minimum energy limitation, appear to be reasonable approaches to the problem. Both methods describe possible events in a lattice, but are they compatable? The general use of the two body approach is desirable because of its simplicity. The problem to be studied is: when can the two body collision be assumed, if at all, and should an "apparent" mass, as proposed by Henschke[8], be employed?

2. Objective.

We intend to investigate theoretically the energy transfer process between an incoming copper atom and a copper lattice. The many body approach, using computer techniques similar to Gibson et. al.[15], will be utilized and then compared with the simple two body solution. We hope the results will provide some quantitative answers to the questions posed in the preceding section.

3. Procedure.

The representative crystal lattice consists of a cube of 63 atoms arranged in a face centered cubic structure. This arrangement gives a total of 63 atoms. These atoms are free to move, if disturbed. In an effort to simulate a larger lattice, the movable 63 atoms are surrounded on all sides by stationary immovable atoms positioned as a continuation of the crystal. This procedure also gives the bombarded face some characteristics similar to a binding energy.

In order to simplify the calculations, we defined a quantity called the "lattice unit". One lattice unit is equal to half the length of a cube side. For copper, the length of a cube side is 3.614A, therefore one lattice unit is 1.807A. A three dimensional Cartesian coordinate system is used for reference with the origin placed with a (100) face of the movable 63 atom "core" parallel to the x-z plane at y=0. Any penetration into the lattice core from this plane is in the + y direction. The immovable atoms surrounding the core are in the x-z plane at y=-1 and y=5, the x-y plane at z=0 and z=6, and the y-z plane at x=0 and x=6. For convenience all atoms are numbered. Number one is the "bullet", numbers 2-64 are the "core" and 65-172 are the immovable atoms.(see Fig. 1)

The program depends upon a potential function subroutine; so potential modification is accomplished without any changes in the main program. The Born-Mayer and the Thomas-Fermi-Firsov have been used in the present work (see Appendix VI for exact forms and constants). All calculations are with the potential in "eroded" form. To "erode" a potential, the value of the potential at the nearest neighbor separation is subtracted from the value of the potential at smaller distances. The eroded form makes the

potential zero at distances greater than nearest neighbors.

The interaction between atoms is represented by an eroded repulsive potential. Also, the entire lattice is initially at absolute zero since no vibrational energy is simulated. These two approximations imply that the lattice has no potential or kinetic energy before interaction with the bullet and all the energy in the lattice at any time thereafter is derived from the bombarding atom.

We realize that each atom in the lattice is contained in some type of "potential well", but we are measuring the energy from the ground state level of this "well" rather than from the true zero of potential at infinite separations. Thus, before interactions with the bullet, our lattice is not held together by the surrounding stationary atoms as in the Gibson et. al.[15] model because the erosion also has removed all forces. Forces appear only when atoms move from their equilibrium positions.

The use of an eroded potential does not provide as good a model as the one used by Gibson et. al., but it reduces the computer time required for calculations.

The "binding energy" created by the layer of fixed atoms covering the front face is probably much too large, but it does approximately simulate the behavior of the next layer of atoms.

The calculations which move atoms are similar to those of Gibson et. al.[15] Newton's equation of motion can be rearranged to give the change in velocity of a body acted on by an unbalanced force. ($F \cdot \Delta T / m = \Delta V$) The change in velocity can be related to a change in position if an average velocity is assumed ($X_{NEW} = \left[V + \frac{\Delta V}{2}\right] \cdot \Delta T + X_{OLD}$). The unbalanced force used in the first equation is an average force calculated by a double iteration procedure as follows: (1) assume an atom at position 1 with velocity 1

(2) calculate the total force on the atom as a result of all the other atoms in the lattice (this means normally only about 8-10 nearest atoms because the potential is eroded) (3) call this calculated force, force 1, and use the equation of motion to move the atom to a temporary position, position 2. (4) now repeat the force calculations for position 2, call this force 2. (5) go back to position 1, and use the average of force 1 and force 2 to move the atom to a new position, position 3. Procedures 1 through 5 constitute one "time step". Forces are eroded in the same manner as potentials and are calculated by a subroutine based on the partial derivative of the potential function with respect to distance.

The basic value of ΔT is dependent upon the original energy of the bombarding atom. ΔT is the time in seconds required for the incoming atom to traverse one lattice unit. The atom will lose energy as it interacts with the lattice but ΔT remains unchanged. To add flexibility to the program, the basic value of ΔT can be multiplied by any desired factor (time step multiplier). ΔT is established at the beginning of the program and is constant for the duration of the calculations.

The bombarding copper atom is originally located in the plane $y = -\sqrt{2}$ and given a velocity in the + y direction only. This requires the bombarding particle to approach perpendicular to the (100) face of the movable lattice core. The immovable atoms in the plane ($y = -1$) that cover the bombarded face do not interact with the bullet.

An impact area was chosen on the (100) face so that all points in this area would be representative of any point in a (100) plane. An impact point is defined as the location on the (100) face toward which the bombarding atom is directed. It may or may not actually pass through this point. By moving in 1/10 lattice unit increments, 36 impact points in the impact "triangle"

were assigned. (see Fig. 2 and 3).

For each case the two body problem is solved after the many body problem with the same double iteration scheme. Lattice atom number eight was assigned as the "target" in the many body lattice problem so that its motion could be compared with the simple two body problem. The geometrical relationship and physical constants of the two body problem correspond to those of the incoming atom and "target" in the crystal.

The program was written in FORTRAN language for use on a CDC 1604 computer. The input consists of the incoming particle mass and energy and the time step multiplier. From these inputs the bullet is assigned a location and an appropriate velocity component in the + y direction. Also calculated is the actual value of ΔT.

The next section of the program assigns coordinates to all atoms in the crystal, movable and immovable, gives each atom a number and sets their velocities equal to zero. If the distance between any two atoms is less than $\sqrt{2}$ lattice units, the force between these two atoms is calculated and stored in memory. This is done for each atom and the summation of all the forces calculated gives the resultant force on each particle.

The change in the velocities of all movable atoms as a result of unbalanced forces is calculated; then the original velocities of all particles and the calculated change in velocity are used to move atoms to temporary locations. The calculations to obtain resultant forces are repeated for the temporary locations, old and new forces are averaged and used to move all atoms to new locations. Forces and velocities are calculated as vector components using the coordinate system established for the lattice.

After each movement of all the atoms, the kinetic energy of the target is calculated and compared to its former value. The procedure is repeated

until the kinetic energy of the target reaches a maximum. The potential and kinetic energy of each movable atom is then calculated. The total energy of the entire lattice including bullet is also found and compared to the original "bullet" energy. This comparison gives a reasonable measure of the accuracy achieved. The two body problem is solved in the next section using the same iteration technique. Appendices I-V contain a detailed explanation of the program.

For each "run", the computer will solve the many body and two body problem 36 times, corresponding to the 36 different impact points. The form of the printed output for each impact point is shown in Fig. 4 and 5. The "triangular" output as seen in Fig. 6 indicates how two chosen parameters vary over the impact area.

The computer running time for each of the 36 impact points was 2-4 minutes, the time varying with the value chosen for ΔT. We originally assumed that the accuracy of the results would increase for smaller and smaller values of ΔT. We found that the value of ΔT which will give the minimum error in total energy appears to be a complicated function of the time step multiplier, the incoming bullet energy, and the impact point. By trial and error methods, we found that below 100 ev for the Born-Mayer potential, a time step multiplier of around 0.09 would produce reasonable errors at all impact points.

4. Potentials

The Born-Mayer potential is an exponential function of the internuclear separation with constants which may be obtained from experimentally measurable elastic moduli. The constants used in the program are the same as those of Gibson et. al.[16], with special emphasis on their potential number two. Near equilibrium separations, the Born-Mayer potential is thought to be an adequate approximation. We expect the potential to fail for energies above a few hundred electron volts.

The Thomas-Fermi-Firsov (TFF) potential is the result of theoretical work by Firsov[17] based on the Thomas-Fermi model of the atom. It is a screened Coulomb potential with a more complicated screening function than that used in the Bohr potential. The TFF is satisfactory for intermediate separations. This places it between the Bohr potential used for small separations and the Born-Mayer potential. Abrahamson and Hatcher[18] state that the Thomas-Fermi approximation becomes unreliable when the internuclear distance exceeds $\sim$1A. The form of the TFF potential and the appropriate constants used in the program are the same as those used in computer programs at the Oak Ridge National Laboratory[19].

The mathematical forms of the potential and force functions as they appear in the program are derived in Appendix VI.

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[16] See reference 15, p. 1233.

[17] O. B. Firsov, J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 1464 (1957). translation: Soviet Phys. -JETP 5, 1192 (1957).

[18] A. A. Abrahamson and R. D. Hatcher, Phys. Rev. 121, 159 (1961).

[19] R. T. Robinson (private communication). The author would like to thank Dr. Robinson for the use of his results prior to their publication.

5. Results

A. General description of events in the lattice.

The number of atoms disturbed in the lattice is a function of two variables, the number of time steps the computer performs and the impact point of the bullet. In general, the lattice is more disrupted by impact points in the area near x = 3.0, z = 4.0, and the lattice is least affected by head on collisions with the target. No more than one half of the atoms were ever disturbed before the target reached a maximum in kinetic energy.

The impact area is not symmetrically located with respect to the surrounding immovable atoms but for appropriate points in the impact area, excellent symmetry of displacement was observed for the movable atoms. This indicates that the size of the model is adequate for present purposes.

Because of the limitation placed on the number of time steps, only a few atoms have any significant kinetic energy when the interaction is stopped. These are normally the target, bullet, and the atoms directly behind the target and bullet in the lattice.

Although our primary purpose was to compare lattice interactions with the two body interaction, we altered the program so that it would run a predetermined number of time steps in order to observe "chains" and "channels". Impact points at x = 3.0, z = 4.0 and x = 3.0, z = 3.0 correspond to the beginning of (100)chains. These are not "close packed" chains but they transfer energy reasonably well, especially above 100 ev. Impact point x = 2.5, z = 3.5 is the beginning of a (100) channel. The (100) channel is not as "wide open" as a (110) channel and a 100 ev bullet does not travel more than $\sim$ 3A into the lattice.

B. Comparison of lattice interactions with the two body interaction.

A strict comparison of interactions in the lattice to the two body problem is not possible, but certain limited correlations can be made. The difficulty arises because the end of the interaction in the lattice cannot be defined explicitly. There are several criteria available that may be used in an attempt to compare the interactions. If the two body interaction was allowed to continue until the potential between atoms was zero, for comparison purposes the lattice interaction could procede until: 1) the potential between target and bullet is equal to zero 2) the total energy (kinetic plus potential) of the target reaches a maximum or 3) the kinetic energy of the target reaches a maximum. All of the criteria apply to the same physical situation in the two body problem but are not equivalent in the lattice interaction.

We chose the maximum kinetic energy of the target as the comparison stopping point because this represents the time when the target and bullet have almost ceased to interact and are just beginning to interact with other lattice atoms.

A fourth criteria was suggested after the present results had been obtained. When the kinetic energy of the target in the lattice reaches a maximum, find the distance between the target and bullet and allow the two body interaction to proceed until the distance between atoms is equal to the separation in the lattice. This criteria is possibly better than the one chosen but at the present time it has not been utilized.

The geometrical relationships of the target, bullet, and lattice introduce complications into the comparison scheme. The motion of the target in the lattice is not restricted isotropically (see Fig. 7). If the interaction with the bullet moves the target toward atom number six (shaded area),

the movement of the target is restricted more than if the target motion is initially toward the cross-hatched area. Restriction of the target motion lengthens the interaction time between bullet and target, therefore the energy transferred to the target is greater than in the two body problem. This effect is noticable only at impact parameters of 0.5 lattice units or greater. At impact distances smaller than this the interaction occurs so rapidly that the target does not move a significant amount and the effect is reduced. The kinetic energy transferred at distances smaller than 0.5 lattice units is less than that transferred in the two body case because there is absorption of energy by the remainder of the lattice. The geometry of the bombarded face is not the only factor that effects energy transfer. The atoms behind the target in the lattice also play an important role but their effect is not as immediately obvious as those just discussed.

Figure 8 illustrates some of the points just mentioned. Along the line A B ($x = 3.0$, $z = 3.0$-4.0) the target behavior in the lattice is similar to the two body interaction. These impact points cause the target to move in the negative z direction toward a "hole" in the lattice face. At point D on the line A C , the effect of restricted target motion becomes obvious, and also in the area enclosed by the dashed line. The geometrical effects of the lattice are fairly predictable and no unusual phenomena are observed.

For a static system of two equal mass atoms with a conservative repulsive force between them, the total potential energy of the system can be halved and the result assigned as the energy of the atom. If the two atoms are allowed to move, the total energy (potential plus kinetic) of each will be constant and equal to the original potential energy. In a system composed of three or more atoms, this is generally not true. For any system where the atoms are not static, the process of assigning an energy to any one atom is

no longer possible (there is one exception). This is the situation in the lattice.

The potential energy of an atom in the lattice is defined in the program as half the potential associated with its position. This definition is merely a convenience.

The area of the impact triangle from point A to the arc E-F (see Fig. 8) is least effected by the geometry of the lattice and closer inspection of these interactions is justified. The kinetic energy transferred to the n-body target is less than that of the two body target. In percentages, the kinetic energy transferred becomes less as the bullet energy is decreased. (see Figs 8 through 11). In each case the target also acquires some potential energy (see Figs. 12 through 15). As stated earlier, it is difficult to assign a specific potential energy to the target. We do know the limits involved, i.e. the target could eventually receive none of it, or twice the indicated value. Either limiting situation is unlikely.

If we make the assumption that one-half of the potential "belongs" to the target, then the total energy of the target is approximately equal to the energy transferred in the two body problem (within 2%) for energies greater than 50 ev.

Bullet behavior for the area under discussion is also very similar to the two body problem (see Figs. 16 through 19). For the remainder of the impact triangle, the bullet is strongly effected by other atoms in the lattice.

Three runs were made with the TFF potential at energies of 5, 10, and 30 kev (Figs. 20 through 25). Since the TFF potential is unreliable beyond 1A, the section ABC in Figs. 20 through 25 is the only part of the impact area that can be considered. This section includes all impact points that

result in a closest point of approach of 1A or less. We noted the same general agreement with the two body interaction as found for the Born-Mayer potential. The only apparent difference is a shift in the energy scale.

For a head-on collision in the lattice there is very little geometrical effect, and an "effective" mass can be described. At 25 ev, the mass of the target is apparently about 2.5 times the bullet mass, but the energy transfer is still approximately 80%. For a 500 ev bullet, the effective mass increase is negligible. We used the program, as modified to observe chains and channels, and could find no evidence of bullet recoil which could be attributed to an effectively heavy target as proposed by Henschke[8]. Although an effective mass concept for the head-on collision is possible, it does not properly describe the subsequent motion of either target or bullet. If the bullet motion results in a glancing hit with the target, no single effective mass can be assigned to the target because it is a function of the impact parameter. An average effective mass is not applicable because the geometrical effects of the lattice on the direction and energy of the recoil atom are far more significant than the mass of the target in a glancing hit.

These results apply to a collision anywhere in the lattice and are not limited to the interaction of surface atoms with incoming particles. The results indicate that Henschke's[8] apparent mass concept and the rebound phenomena associated with it are not a good description of collision events in a lattice.

6. Conclusions

A. The Bullet.

For energies above 40 ev in the impact area AEF (see Figs 16 and 17), the n-body bullet's kinetic energy after interaction is essentually the same as the two body bullet. Between 40 and 400 ev for impact points outside the area AEF, the n-body bullet has considerably less energy after interaction than the two body bullet. Above 400 ev, the n-body and two body energy transfers agree within 3% for all points in the impact area.

The angular behavior of a bullet in the lattice is much more complicated. Even at energies above 400 ev, the scattering angle in the n-body problem is affected by the geometry of the lattice. In general, the scattering angle in the lattice is smaller than that of the two body problem. It is possible that the lattice is attempting to focus the energy into preferred directions. Our bullets in the (100) direction appear to focus in the (100) direction, especially at higher energies.

The cummulative effects of energy transfer and lattice geometry will affect the range of energetic atoms. The reduced scattering angle in the n-body model for atoms with energies above 400 ev should lead to ranges that exceed those found by two body approximation methods. Below 400 ev, the bullet loses more energy than in the two body case; so the effects may cancel, or perhaps ranges calculated by two body methods may be too large.

B. The Target.

In the area AEF (see Figs. 8, 9, 12, 13), the n-body energy transferred to the target is the same (within 2%) as that in the two body problem for energies above 50 ev. For the remainder of the impact area, the n-body target receives more energy than the two body target for all energies above

25 ev. Isolated points at various energies may not conform to this rule but the effect is always present for impact points near the apex of the impact area (x=2.5, z=3.5). Near the apex, if the bullet energy is large (300 ev or greater), the energy transferred to the target is a very small fraction of the total for both the n-body and two body problems. However, the energy transferred to the target in the two cases can differ by as much as 75% of the transferred energy.

As a consequence of this phenomena, the low energy portion of the n-body target atom energy distribution (assuming more than one collision has occurred) will be much higher than that expected with a two body collision assumption for lattice interactions. Precise measurements of energy transfer for large impact parameters do not appear to be warranted in view of the results obtained.

Unfortunately, the face centered cubic lattice structure was incorporated in the program before we learned of Veksler's[20] experimental work with molybdenum targets (bcc), but certain qualitative comparisons are still possible. Veksler has interpreted the lattice behavior in terms of the effective mass concept but his general conclusions are consistent with our work. Our model gives good evidence to support Veksler's position that the pair collision model using elastic spheres is not acceptable.

Two body approximations inherently imply that certain information is available from preliminary n-body calculations. This work attempts to answer certain questions about interactions and cross sections. As anticipated, the results are not definitive but they do indicate sensitive areas which require further examination.

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[20] V. I. Veksler, J. Exptl. Theoret. Phys. (U.S.S.R.) 42, 325 (1962). translation: Soviet Physics - JETP 15, 222 (1962).

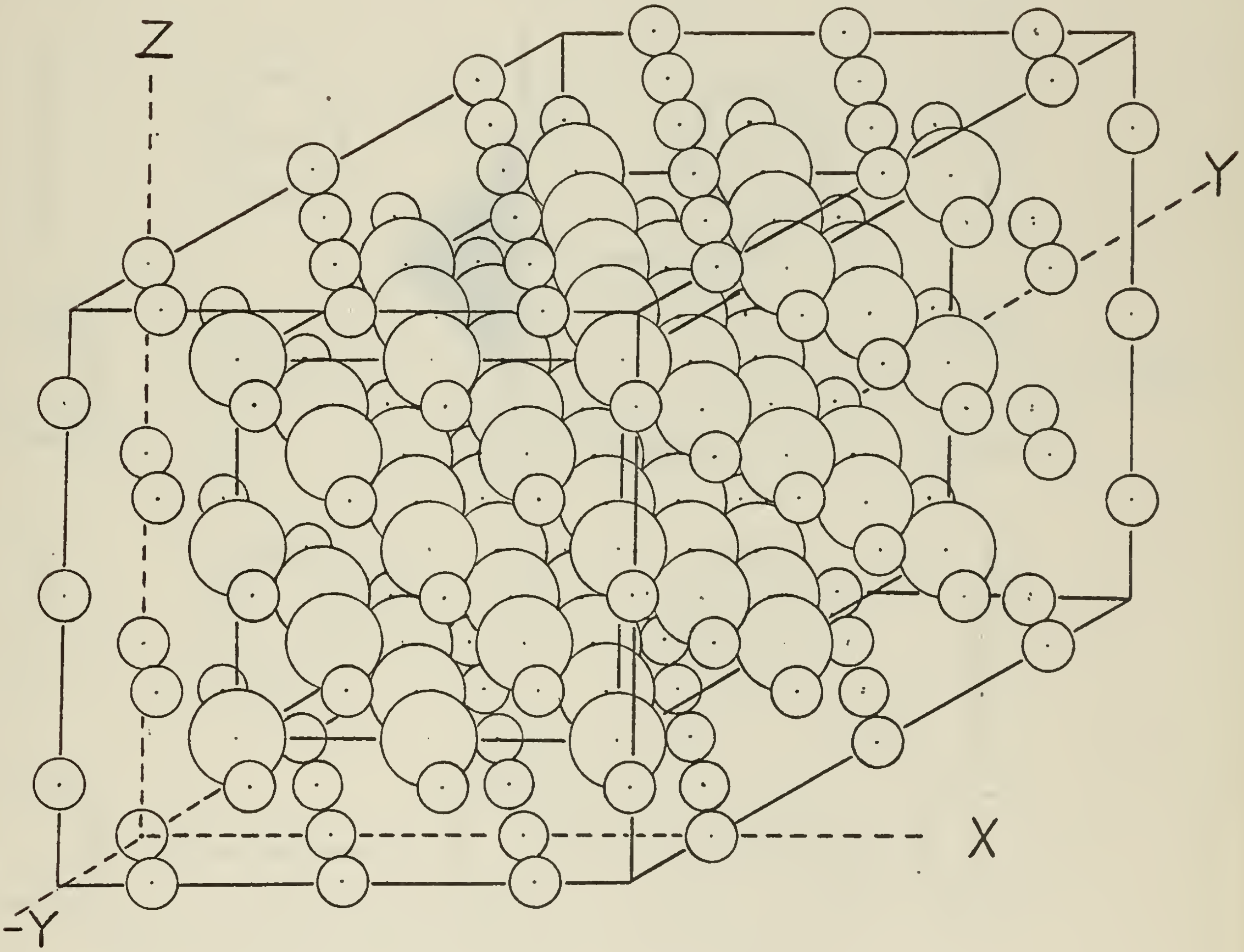


Fig. 1. THE MODEL
Large circles indicate movable atoms;
small circles indicate fixed atoms.

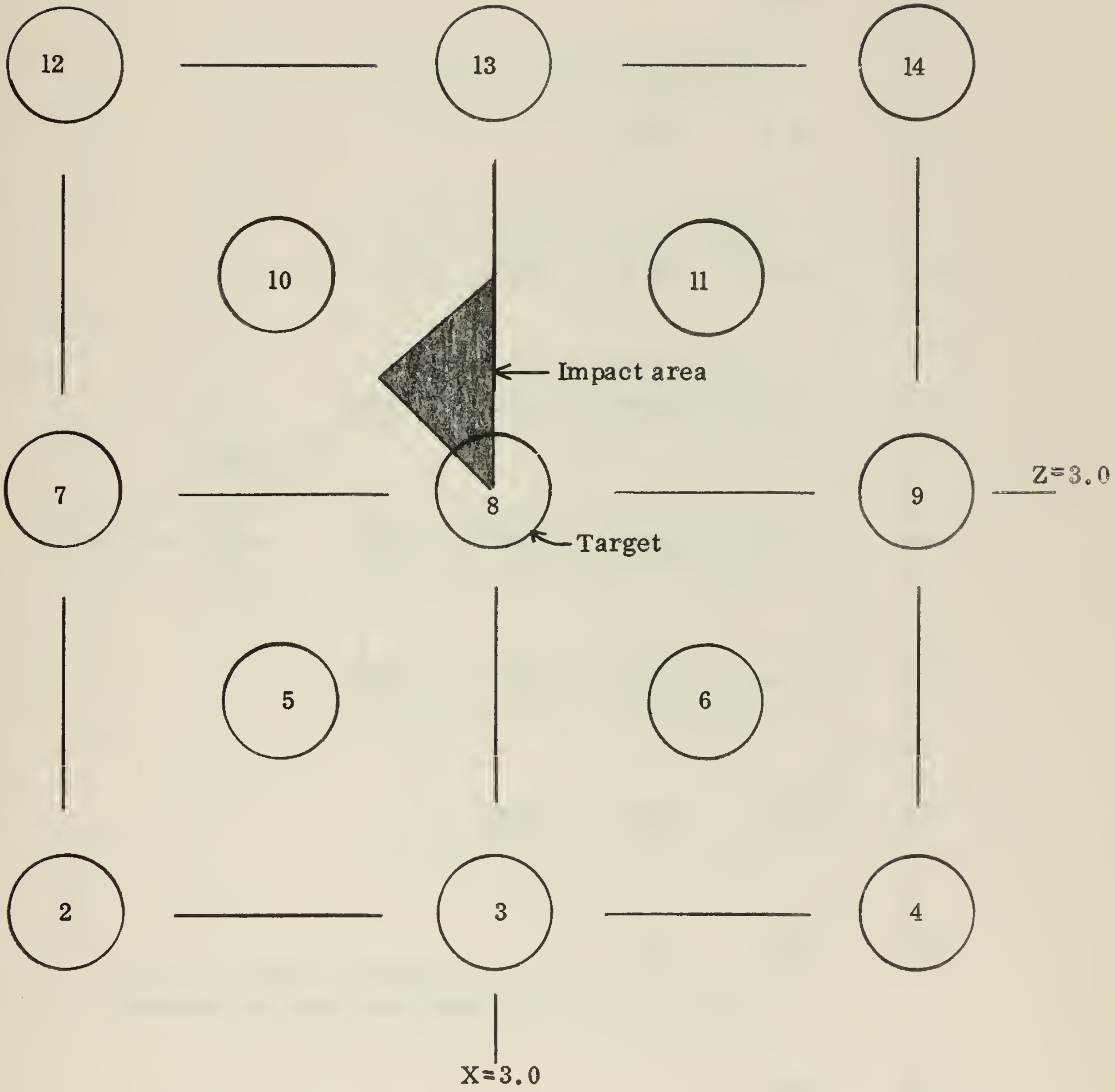


Fig. 2. FACE (100) of LATTICE CORE.
Numbers indicate atoms; shaded portion is impact area

[illegible]

[illegible]

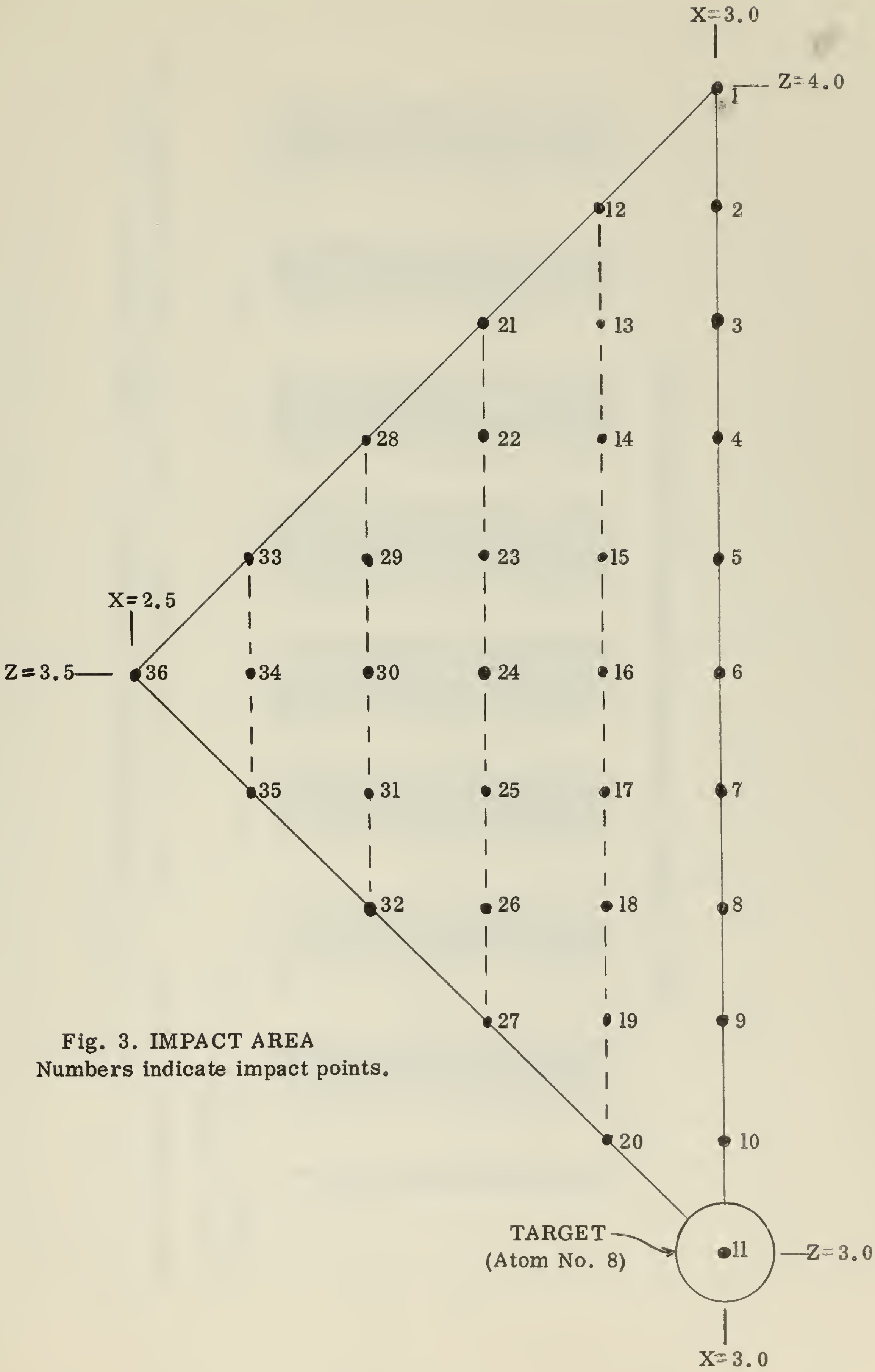


Fig. 3. IMPACT AREA
Numbers indicate impact points.

```
                         BORN-MAYER ERODED POTENTIAL       COPPER LATTICE AND BULLET
BULLET INCOMING LOCATION  X= 3.000   Z= 3.900   ENERGY=    100.0   TIME STEP MULTIPLIER= .080

LATTICE LOCATIONS
 ATOM        DX         DY         DZ         VX         VY         VZ         KE         PE

    1     .00000    1.90693     .00294    .00E+00    .49E+03    .16E+03     .08939    1.50805
    6     .00056    -.00001    -.00052    .25E+02   -.59E+00   -.22E+02     .00037     .04162
    8     .00000     .02941    -.15781    .00E+00    .21E+03   -.25E+04    2.00737     .30768
    9     .00019    -.00000    -.00020    .84E+01   -.67E-01   -.88E+01     .00005     .01459
   10    -.07887     .00832     .00659   -.14E+04   -.19E+02    .10E+03     .62477     .25087
   11     .07887     .00832     .00659    .14E+04   -.19E+02    .10E+03     .62477     .25087
   12    -.00024    -.00000     .00025   -.10E+02   -.83E-01    .11E+02     .00007     .01827
   13     .00000     .00152     .04014    .00E+00   -.72E+02    .78E+03     .20369     .21268
   14     .00024    -.00000     .00025    .10E+02   -.83E-01    .11E+02     .00007     .01827
   18     .00000     .00079    -.00074    .00E+00    .35E+02   -.32E+02     .00072     .05698
   20    -.00013     .00016    -.00002   -.38E+01    .44E+01   -.30E+00     .00001     .00289
   21     .00013     .00016    -.00002    .38E+01    .44E+01   -.30E+00     .00001     .00289
   22    -.00028     .00028    -.00000   -.11E+02    .12E+02   -.51E-01     .00009     .01884
   23     .00000     .52157     .04273    .00E+00    .17E+05    .13E+04   90.52631    2.40895
   24     .00028     .00028    -.00000    .11E+02    .12E+02   -.51E-01     .00009     .01884
   25    -.00002     .00008     .00007   -.52E+00    .25E+01    .23E+01     .00000     .00213
   26     .00002     .00008     .00007    .52E+00    .25E+01    .23E+01     .00000     .00213
   33     .00000     .00055    -.00077    .00E+00    .48E+02   -.78E+02     .00276     .26470
   35    -.00096     .00068    -.00002   -.10E+03    .63E+02   -.32E+01     .00481     .38456
   36     .00096     .00068    -.00002    .10E+03    .63E+02   -.32E+01     .00481     .38456
   38     .00000     .00086     .00119    .00E+00    .85E+02    .14E+03     .00846     .56089
```

Fig. 4. TYPICAL COMPUTER OUTPUT for an impact point

```
                       BORN-MAYER ERODED POTENTIAL      COPPER LATTICE AND BULLET
BULLET INCOMING LOCATION  X= 3.000   Z= 3.900   ENERGY=   100.0   TIME STEP MULTIPLIER= .080


RESULTS OF SIMPLE TWO BODY INTERACTION
KIN ENRG PROJ= 98.293220    KIN ENRG TARG=     1.70688    TOT ENRG=    100.00010    ENRG IN=   100.00000


RESULTS OF LATTICE INTERACTIJN
TARGET VALUES
 TIME STEPS    POT E TARGET W/R TOBULLET    KE TARGET    POT E TARGET W/R TO LAT-BULLET
     32.                   .269015          2.007372                        .000000
BULLET VALUES
  KIN ENERGY =   .089    POT E W/R TO LAT-TARGET =  1.369    VELOCITY IN M/SEC  X=  .00E-01  Y= 4.95E+02  Z= 1.64E+02
LATTICE VALUES
    POT ENERGY      KIN ENERGY     TOT  ENERGY     PER ERROR
       6.87605        94.09908      100.97512     .97512

COMPARISON VALUES OF LATTICE REACTION AGAINST SIMPLE TWO BODY PROBLEM
BOTH INTERACTIONS STOPPED WHEN TARGET KINETIC ENERGY MAXIMUM
  PERCENT KE TRANSFERED          TWO BODY=    1.707          LATTICE=    2.007
  RATIO KE TRANSFER IN LATTICE / KE TRANSFER TWO BODY =1.17605
  RATIO KE PROJ IN LATTICE / KE PROJ TWO BODY =     .00091
  RATIO BULLET MASS / TARGET MASS = 1.000
  POT + KE ABSORBED BY LATTICE =  97.06764
  SCATTERING ANGLE          TWO BODY =   7.51          LATTICE =  18.29
  RECOIL ANGLE          TWO BODY =  82.49          LATTICE =  85.02
  RATIO SCATTERING ANGLE TWO BODY / SCATTERING ANGLE LATTICE =   .41035
  RATIO RECOIL ANGLE TWO BODY / RECOIL ANGLE LATTICE =   .97033
  IMPACT PARAMETER =  .9000     RATIO KE BULLET AT END OF RUN / ORIGINAL ENERGY =  8.93871E-04
```

Fig. 5. TYPICAL COMPUTER OUTPUT for an impact point

```
                              BORN-MAYER ERODED POTENTIAL        COPPER LATTICE AND BULLET
              BULLET INCOMING ENERGY = 100.0  EV       TIME STEP MULTIPLIER = .080       BULLET INCIDENT ON (100) FACE

                                      TOP NO. IS KINETIC ENERGY IN EV OF BULLET IN LATTICE
                                      BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE

            B                                                                                                        C
                                 (Z = 3.8)                         (Z=3.5)                        (Z=3.2)
           .124       .089       7.926     56.201     63.901     56.194     41.205     25.710     12.326      3.241      .008
  (X=3.0)   *          *          *          *          *          *          *          *          *          *          *
           .710       2.007      5.402     12.281     23.131     37.294     53.160     68.855     82.443     91.836     95.244
                                                                                                 (3.0, 3.0) TARGET ATOM

                      .067       8.557     42.977     63.319     55.258     41.338     27.368     14.870      6.298
            (X=2.9)    *          *          *          *          *          *          *          *          *
                      1.972      5.279     11.944     22.418     36.018     51.345     66.467     79.645     88.624


                      (X=2.8)    4.380     45.648     61.492     50.686     38.213     29.733     21.749
                                  *          *          *          *          *          *          *
                                 5.104     11.263     20.651     32.704     46.255     59.924     71.643


                               (X=2.7)    23.435     50.628     46.253     32.967     33.076
                                            *          *          *          *          *
                                          11.135     19.085     28.664     39.279     50.190


                                        (X=2.6)      45.033     43.875     36.110
                                                       *          *          *
                                                     19.221     25.491     32.090


                                                  (X= 2.5)      43.295
                                                                  *
                                                                23.701
                                                                  A
```

Fig. 6. TRIANGULAR COMPUTER OUTPUT; (*) indicates impact point

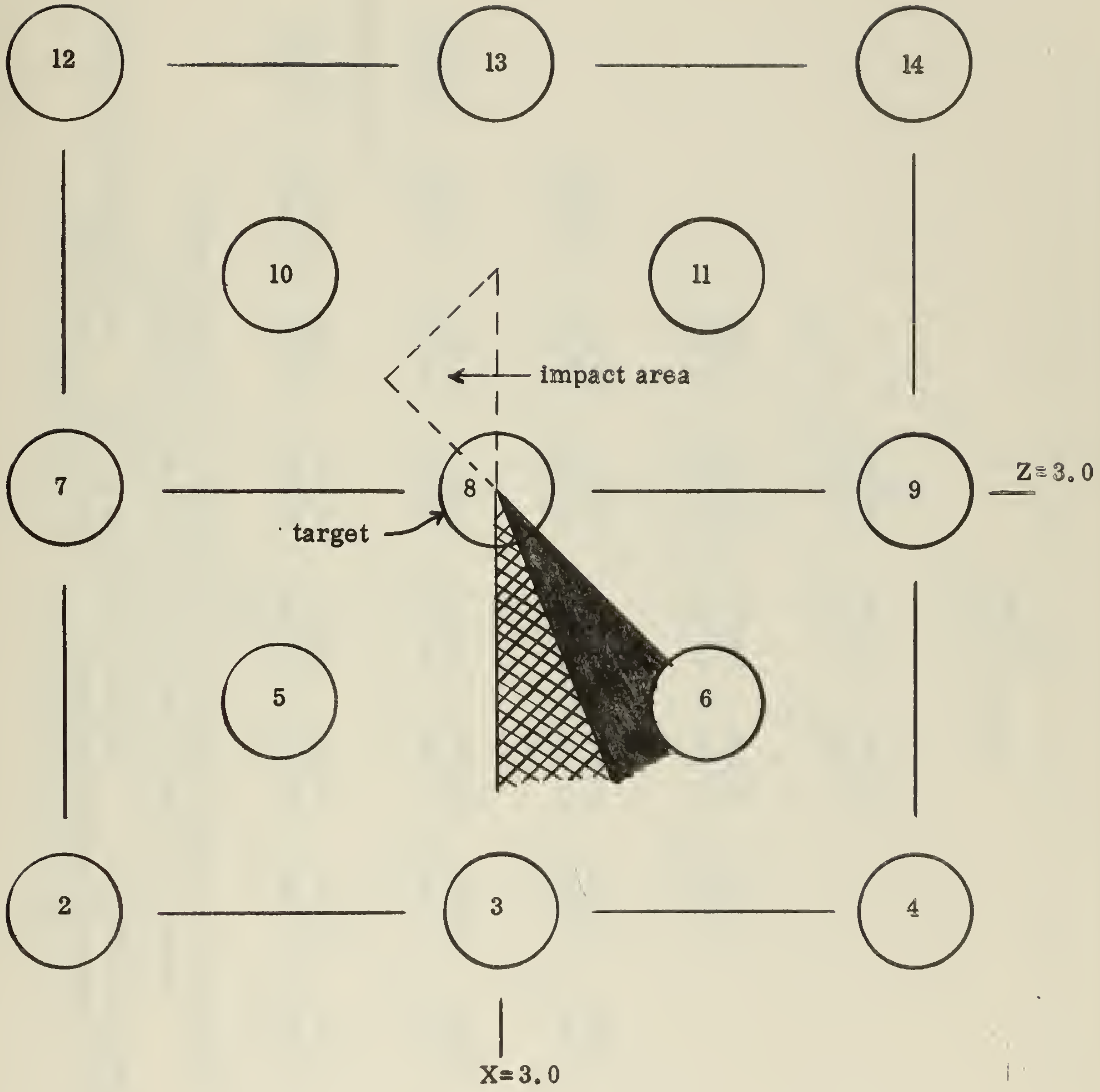
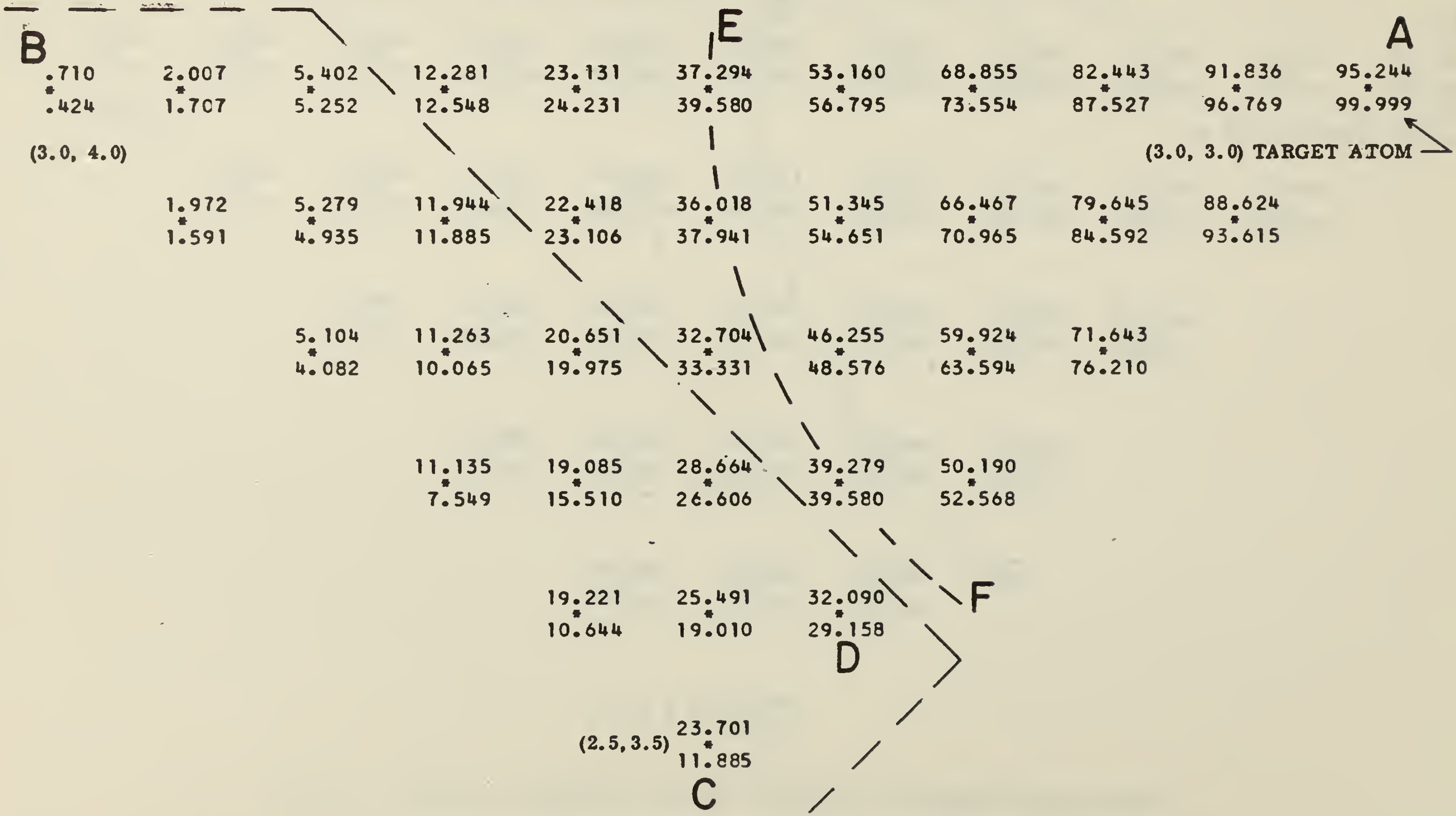


Fig. 7. GEOMETRICAL EFFECTS OF THE LATTICE FACE. Target movement is more restricted if initial motion is in shaded area rather than in crosshatched area.

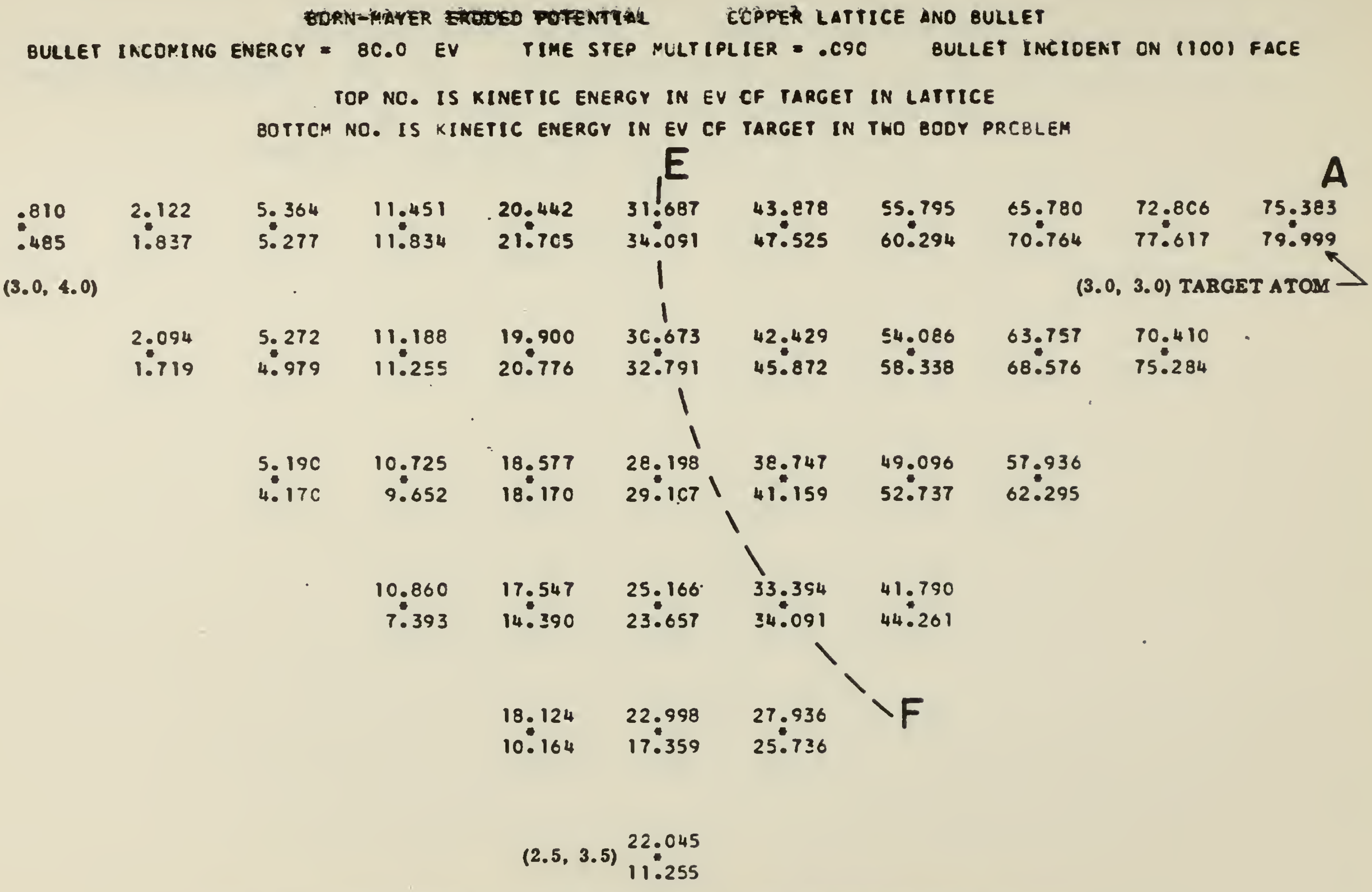
[illegible]

```
                BORN-MAYER ERODED POTENTIAL       COPPER LATTICE AND BULLET
     BULLET INCOMING ENERGY = 100.0  EV     TIME STEP MULTIPLIER = .080     BULLET INCIDENT ON (100) FACE

                    TOP NO. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE
                 BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN TWO BODY PROBLEM
```



```
 .710    2.007    5.402   12.281   23.131   37.294   53.160   68.855   82.443   91.836   95.244
  *        *        *        *        *        *        *        *        *        *        *
 .424    1.707    5.252   12.548   24.231   39.580   56.795   73.554   87.527   96.769   99.999


         1.972    5.279   11.944   22.418   36.018   51.345   66.467   79.645   88.624
           *        *        *        *        *        *        *        *        *
         1.591    4.935   11.885   23.106   37.941   54.651   70.965   84.592   93.615


                  5.104   11.263   20.651   32.704   46.255   59.924   71.643
                    *        *        *        *        *        *        *
                  4.082   10.065   19.975   33.331   48.576   63.594   76.210


                          11.135   19.085   28.664   39.279   50.190
                             *        *        *        *        *
                           7.549   15.510   26.606   39.580   52.568


                                   19.221   25.491   32.090
                                      *        *        *
                                   10.644   19.010   29.158


                                            23.701
                                               *
                                            11.885
```

Fig. 8. GEOMETRICAL EFFECTS on 100 ev bullet; (*) indicates impact point



```
                    BORN-MAYER ERODED POTENTIAL        COPPER LATTICE AND BULLET
BULLET INCOMING ENERGY =  80.0   EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                          TOP NO. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE
                      BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN TWO BODY PROBLEM

 .810    2.122    5.364   11.451   20.442   31.687   43.878   55.795   65.780   72.806   75.383
   *       *        *        *        *        *        *        *        *        *        *
 .485    1.837    5.277   11.834   21.705   34.091   47.525   60.294   70.764   77.617   79.999

(3.0, 4.0)                                                              (3.0, 3.0) TARGET ATOM

         2.094    5.272   11.188   19.900   30.673   42.429   54.086   63.757   70.410
           *        *        *        *        *        *        *        *        *
         1.719    4.979   11.255   20.776   32.791   45.872   58.338   68.576   75.284


                  5.190   10.725   18.577   28.198   38.747   49.096   57.936
                    *        *        *        *        *        *        *
                  4.170    9.652   18.170   29.107   41.159   52.737   62.295


                          10.860   17.547   25.166   33.394   41.790
                             *        *        *        *        *
                           7.393   14.390   23.657   34.091   44.261


                                   18.124   22.998   27.936
                                      *        *        *
                                   10.164   17.359   25.736


                         (2.5, 3.5) 22.045
                                       *
                                    11.255
```

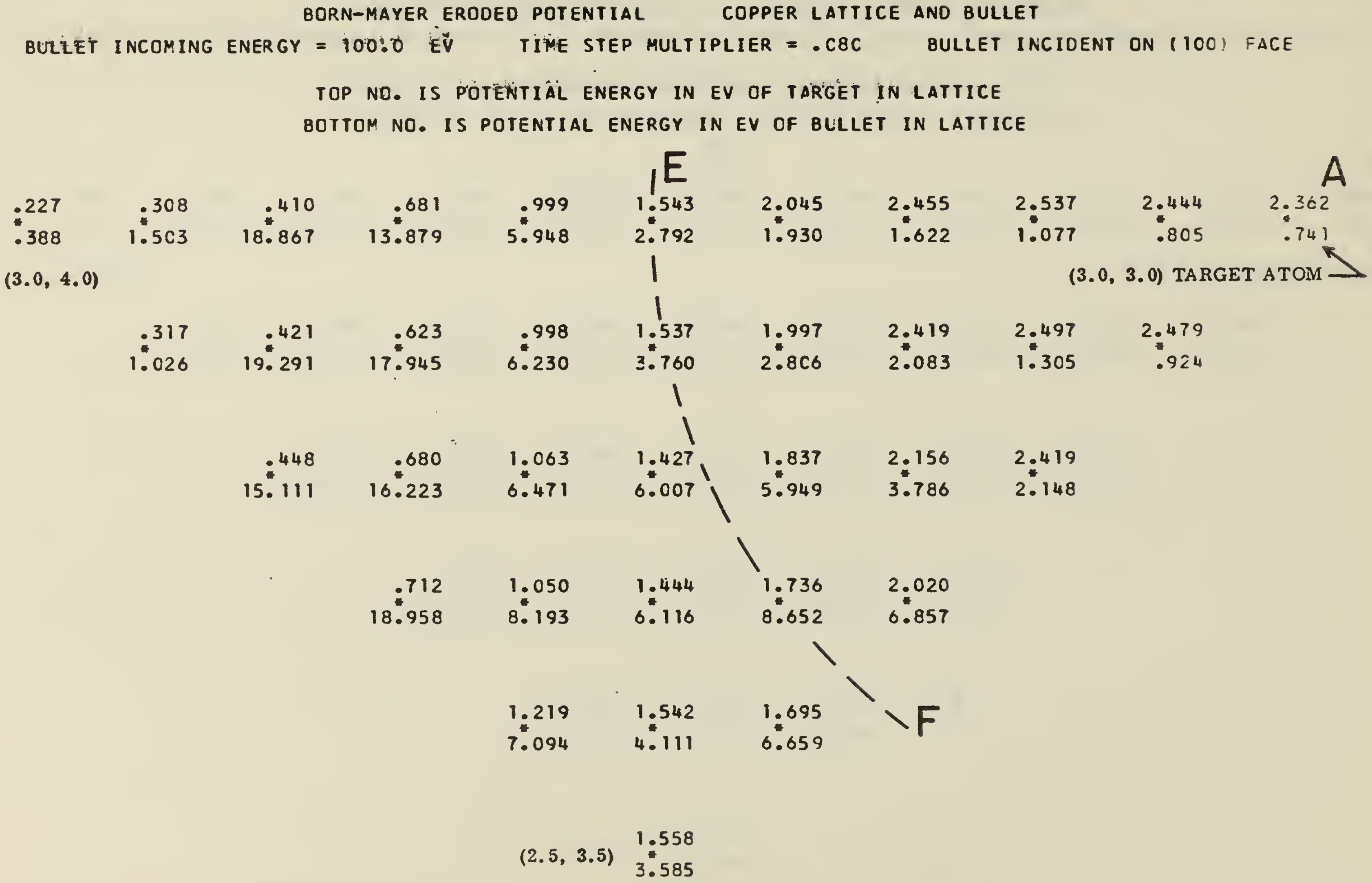
Fig. 9. OUTPUT TRIANGLE for 80 ev bullet; (*) indicates impact point

```
                BCRN-MAYER ERODEC POTENTIAL        COPPER LATTICE AND BULLET
 BULLET INCOMING ENERGY =  4C.C  EV      TIME STEP MULTIPLIER = .09C      BULLET INCIDENT ON (1CC) FACE

                      TOP NC. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE
                   BOTTCM NO. IS KINETIC ENERGY IN EV CF TARGET IN TWC BODY PRCBLEM

                                                     E                                                  A
 1.124     2.28C     4.663     8.347    13.C44    18.329    23.791    28.724    32.936    35.703    36.683
   *         *         *         *        *         *         *         *         *         *         *
  .666     2.C46     4.778     8.998    14.422    2C.494    26.567    32.017    36.314    39.057    4C.CCO
(3.0, 4.0)                                                                        (3.0, 3.0) TARGET ATOM

           2.277     4.647     8.239    12.8C4    17.926    23.206    27.946    32.074    34.762
             *         *         *        *         *         *         *         *         *
           1.937     4.563     8.653    13.940    19.882    25.841    31.198    35.427    38.129

                     4.713     8.125    12.218    16.797    21.496    25.962    29.579
                       *         *        *         *         *         *         *
                     3.964     7.676    12.560    18.119    23.741    28.823    32.849

                               8.459    11.923    15.466    19.180    22.846
                                 *        *         *         *         *
                               6.231    10.478    15.420    2C.494    25.128

                                        12.459    14.615    16.730          F
                                          *         *         *
                                         7.992    12.122    16.465

                                                   14.356
                                      (2.5,3.5)      *
                                                    8.653
```

Fig. 10. OUTPUT TRIANGLE for 40 ev bullet; (*) indicates impact point

```
                  BORN-MAYER ERODED POTENTIAL       COPPER LATTICE AND BULLET
   BULLET INCOMING ENERGY =  25.0  EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                         TOP NO. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE
                     BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN TWO BODY PROBLEM

                                                     E                                                  A
 1.271     2.144     3.824     6.224     9.066    12.172    15.313    17.998    20.327    21.822    22.345
  *         *         *         *         *         *         *         *         *         *         *
  .749     1.988     4.095     6.999    10.441    14.082    17.582    20.637    23.000    24.491    25.000
(3.0, 4.0)                                                                            (3.0, 3.0) TARGET ATOM

           2.154     3.817     6.170     8.937    11.948    14.980    17.584    19.852    21.316
            *         *         *         *         *         *         *         *         *
           1.897     3.939     6.772    10.144    13.723    17.170    20.182    22.515    23.987

                     3.891     6.079     8.613    11.306    13.999    16.500    18.464
                      *         *         *         *         *         *         *
                     3.496     6.118     9.285    12.678    15.968    18.855    21.097

                               6.270     8.375    10.447    12.634    14.754
                                *         *         *         *         *
                               5.128     7.963    11.052    14.082    16.763

                                         8.544     9.830    11.130
                                          *         *         *          F
                                         6.331     9.010    11.686

                                                   9.511
                                      (2.5, 3.5)    *
                                                   6.772
```

Fig. 11. OUTPUT TRIANGLE for 25 ev bullet; (*) indicates impact point



```
                         BORN-MAYER ERODED POTENTIAL       COPPER LATTICE AND BULLET
BULLET INCOMING ENERGY = 100.0  EV      TIME STEP MULTIPLIER = .C8C      BULLET INCIDENT ON (100) FACE

                         TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LATTICE
                         BOTTOM NO. IS POTENTIAL ENERGY IN EV OF BULLET IN LATTICE

 .227      .308      .410      .681      .999     1.543     2.045     2.455     2.537     2.444     2.362
  *         *         *         *         *         *         *         *         *         *         *
 .388     1.503    18.867    13.879     5.948     2.792     1.930     1.622     1.077      .805      .741
(3.0, 4.0)                                                                    (3.0, 3.0) TARGET ATOM

           .317      .421      .623      .998     1.537     1.997     2.419     2.497     2.479
            *         *         *         *         *         *         *         *         *
          1.026    19.291    17.945     6.230     3.760     2.8C6     2.083     1.305      .924


                     .448      .680     1.063     1.427     1.837     2.156     2.419
                      *         *         *         *         *         *         *
                   15.111    16.223     6.471     6.007     5.949     3.786     2.148


                               .712     1.050     1.444     1.736     2.020
                                *         *         *         *         *
                             18.958     8.193     6.116     8.652     6.857


                                         1.219     1.542     1.695
                                          *         *         *
                                         7.094     4.111     6.659


                                     (2.5, 3.5)  1.558
                                                  *
                                                 3.585
```

Fig. 12. OUTPUT TRIANGLE for 100 ev bullet; (*) indicates impact point

```
                     BORN-MAYER ERODED POTENTIAL      COPPER LATTICE AND BULLET
  BULLET INCOMING ENERGY =  8C.C  EV     TIME STEP MULTIPLIER = .C9C     BULLET INCIDENT CN (100) FACE

                     TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LATTICE
                     BCTTOM NO. IS POTENTIAL ENERGY IN EV OF BULLET IN LATTICE

                                             E                                             A
  .246     .309     .440     .691     1.023    1.558    2.020    2.251    2.415    2.331    2.244
   *        *        *        *        *        *        *        *        *        *        *
  .381     2.7C6    18.C90   9.854    4.429    2.504    1.927    1.187    .745     .529     .485

(3.0, 4.0)                                                                 (3.0, 3.0) TARGET ATOM

           .317     .455     .713     1.022    1.568    2.015    2.179    2.358    2.362
            *        *        *        *        *        *        *        *        *
           2.825    18.027   9.550    4.759    3.354    2.587    1.6C8    .944     .629

                    .471     .699     1.086    1.425    1.758    2.063    2.214
                     *        *        *        *        *        *        *
                    15.665   11.69C   5.129    5.333    4.914    3.C76    1.695

                             .786     1.165    1.458    1.684    1.850
                              *        *        *        *        *
                             11.995   4.8C4    5.352    7.498    6.137

                                      1.300    1.613    1.686         F
                                       *        *        *
                                      4.843    3.756    5.916

                             (2.5, 3.5)        1.665
                                                *
                                               2.569
```

Fig. 13. OUTPUT TRIANGLE for 80 ev bullet; (*) indicates impact point

```
                   BORN-MAYER ERODED POTENTIAL       COPPER LATTICE AND BULLET
   BULLET INCOMING ENERGY =  40.0  EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                   TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LATTICE
                   BOTTOM NO. IS POTENTIAL ENERGY IN EV OF BULLET IN LATTICE

 .309     .362     .504     .747     1.011    1.315    1.558    1.773    1.773    1.753    1.738
   *        *        *        *        *        *        *        *        *        *        *
 .795     7.998    7.615    3.644    2.414    1.622    1.142    1.132    .807     .650     .619
(3.0, 4.0)                                                                  (3.0, 3.0) TARGET ATOM

          .373     .520     .771     1.014    1.293    1.530    1.770    1.769    1.762
            *        *        *        *        *        *        *        *        *
          8.065    7.186    3.546    2.720    2.159    1.535    1.322    .916     .717

                   .542     .782     1.074    1.286    1.498    1.624    1.762
                     *        *        *        *        *        *        *
                   7.176    3.414    3.153    3.415    2.740    1.732    1.282

                            .879     1.151    1.311    1.411    1.528
                              *        *        *        *        *
                            2.859    2.443    3.573    4.281    3.085

                                     1.325    1.441    1.427
                                       *        *        *
                                     1.655    2.435    3.877

                             (2.5, 3.5) 1.545
                                          *
                                        1.612
```

Fig. 14. OUTPUT TRIANGLE for 40 ev bullet; (*) indicates impact point

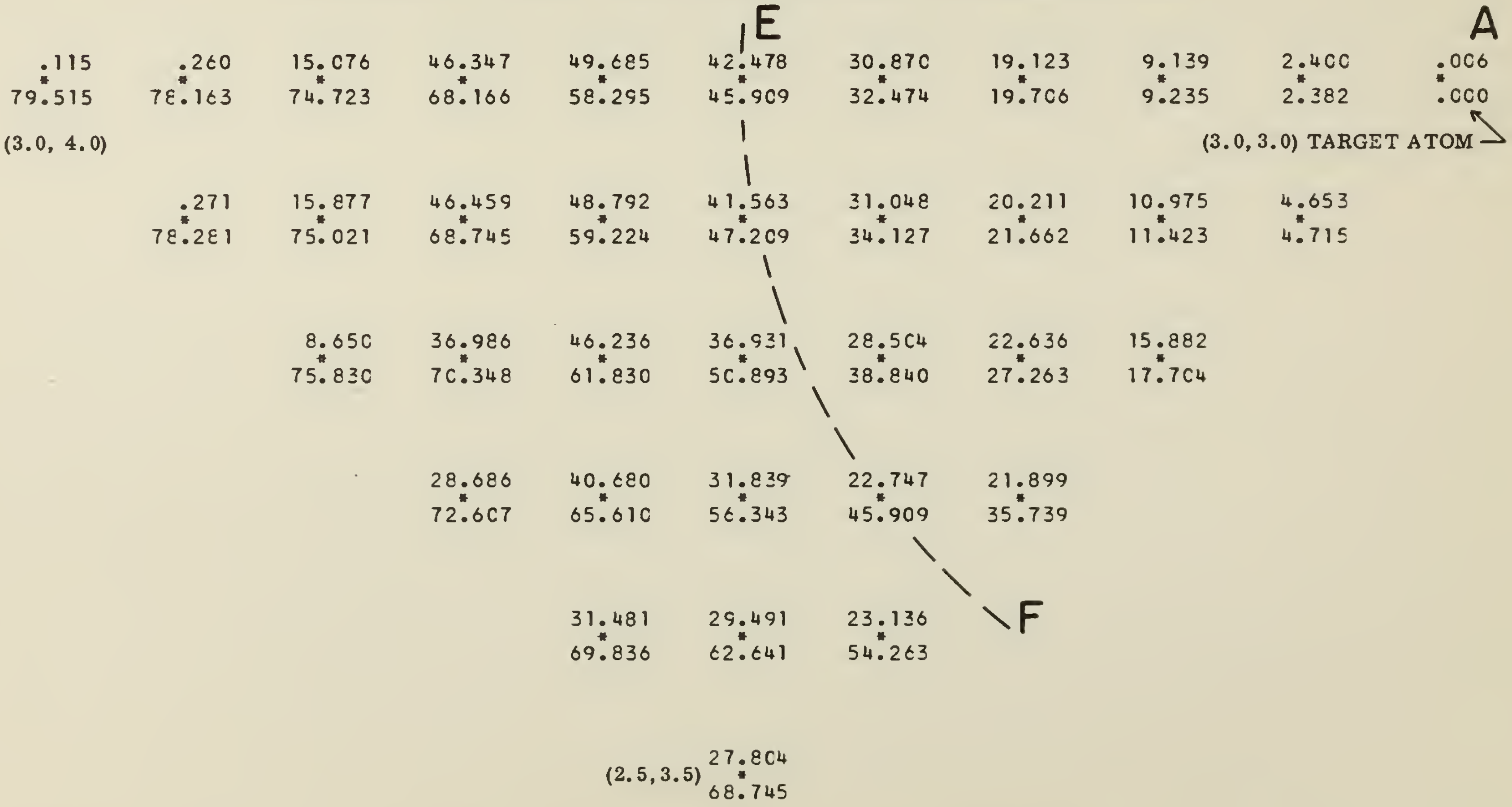
```
                    BORN-MAYER ERODED POTENTIAL          COPPER LATTICE AND BULLET
      BULLET INCOMING ENERGY =  25.0  EV      TIME STEP MULTIPLIER = .C90      BULLET INCIDENT ON (1CO) FACE

                         TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LATTICE
                         BOTTOM NC. IS POTENTIAL ENERGY IN EV OF BLLLET IN LATTICE


   .353     .4C0     .559     .719     .996    1.159    1.315    1.476    1.470    1.464    1.460
    *        *        *        *        *        *        *        *        *        *        *
  1.954    5.453    3.603    2.554    1.821    1.187     .872     .916     .674     .566     .541
(3.0, 4.0)                                                                 (3.0, 3.0) TARGET ATOM

            .4C8     .543     .732     .938    1.138    1.295    1.449    1.469    1.467
             *        *        *        *        *        *        *        *        *
           5.347    3.878    2.442    1.991    1.535    1.116     .674     .754     .609


                     .585     .795     .959    1.115    1.268    1.364    1.469
                      *        *        *        *        *        *        *
                    3.091    2.1CC    2.233    2.337    1.860    1.174     .998


                              .855    1.C25    1.144    1.213    1.290
                               *        *        *        *        *
                             1.469    1.604    2.367    2.760    2.014


                                       1.139    1.228    1.228
                                        *        *        *
                                        .989    1.560    2.517


                              (2.5, 3.5) 1.288
                                          *
                                          .962
```

Fig. 15. OUTPUT TRIANGLE for 25 ev bullet; (*) indicates impact point

```
                      BORN-MAYER ERODED POTENTIAL       COPPER LATTICE AND BULLET
 BULLET INCOMING ENERGY = 100.0  EV      TIME STEP MULTIPLIER = .080      BULLET INCIDENT ON (100) FACE

                        TOP NO. IS KINETIC ENERGY IN EV OF BULLET IN LATTICE
                     BOTTOM NO. IS KINETIC ENERGY IN EV OF BULLET IN TWOBODY PROBLEM

                                                  E                                                 A
   .124      .089     7.926    56.201    63.901    56.194    41.205    25.710    12.326    3.241     .008
     *         *        *         *         *         *         *         *         *        *         *
 99.576    98.293    94.748    87.452    75.769    60.420    43.205    26.445    12.472    3.230     .000
(3.0, 4.0)                                                                        (3.0,3.0) TARGET ATOM

             .067     8.557    42.977    63.319    55.258    41.338    27.368    14.870    6.298
               *        *         *         *         *         *         *         *        *
           98.409    95.065    88.115    76.894    62.058    45.348    29.034    15.407    6.384

                      4.380    45.648    61.492    50.686    38.213    29.733    21.749
                        *         *         *         *         *         *         *
                     95.918    89.935    80.024    66.669    51.423    36.406    23.789

                               23.435    50.628    46.253    32.967    33.076
                                  *         *         *         *         *
                               92.452    84.490    73.393    60.420    47.432

                                         45.033    43.875    36.110       F
                                            *         *         *
                                         89.356    80.990    70.842

                                        (2.5, 3.5) 43.295
                                                      *
                                                   88.115
```

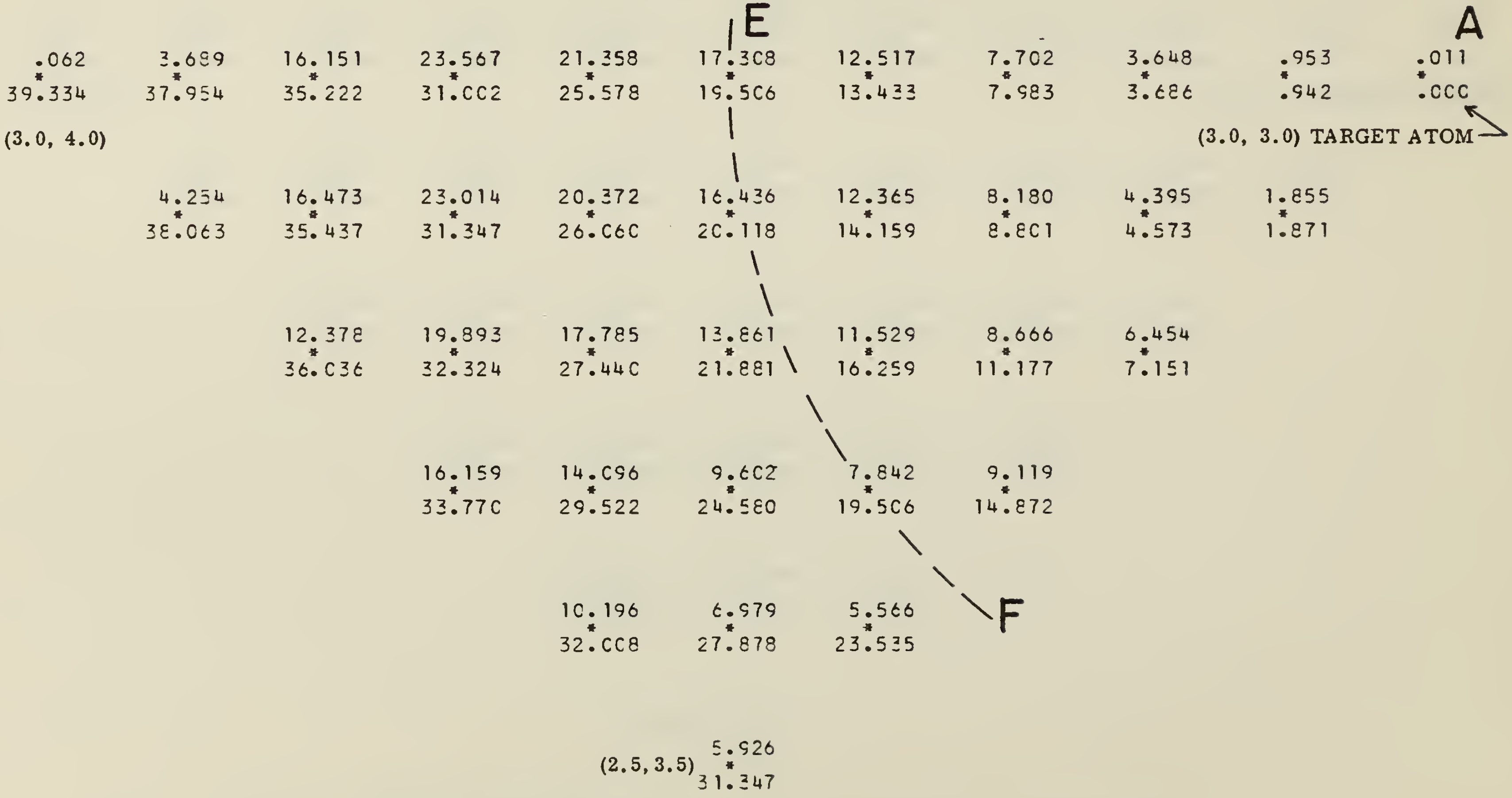
Fig. 16. OUTPUT TRIANGLE for 100 ev bullet; (*) indicates impact point

```
                 BORN-MAYER ERODED POTENTIAL      COPPER LATTICE AND BULLET
BULLET INCOMING ENERGY =  80.0  EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                 TOP NO. IS KINETIC ENERGY IN EV OF BULLET IN LATTICE
              BOTTOM NO. IS KINETIC ENERGY IN EV OF BULLET IN TWOBODY PROBLEM
```



```
                                              E                                                 A
  .115     .260    15.076   46.347   49.685   42.478   30.870   19.123    9.139    2.400     .006
   *        *        *        *        *        *        *        *        *        *        *
79.515   78.163    74.723   68.166   58.295   45.909   32.474   19.706    9.235    2.382     .000
(3.0, 4.0)                                                                (3.0,3.0) TARGET ATOM

           .271    15.877   46.459   48.792   41.563   31.048   20.211   10.975    4.653
            *        *        *        *        *        *        *        *        *
         78.281    75.021   68.745   59.224   47.209   34.127   21.662   11.423    4.715

                    8.650   36.986   46.236   36.931   28.504   22.636   15.882
                     *        *        *        *        *        *        *
                   75.830   70.348   61.830   50.893   38.840   27.263   17.704

                            28.686   40.680   31.839   22.747   21.899
                              *        *        *        *        *
                            72.607   65.610   56.343   45.909   35.739

                                     31.481   29.491   23.136         F
                                       *        *        *
                                     69.836   62.641   54.263

                                     (2.5,3.5) 27.804
                                                 *
                                               68.745
```

Fig. 17. OUTPUT TRIANGLE for 80 ev bullet; (*) indicates impact point



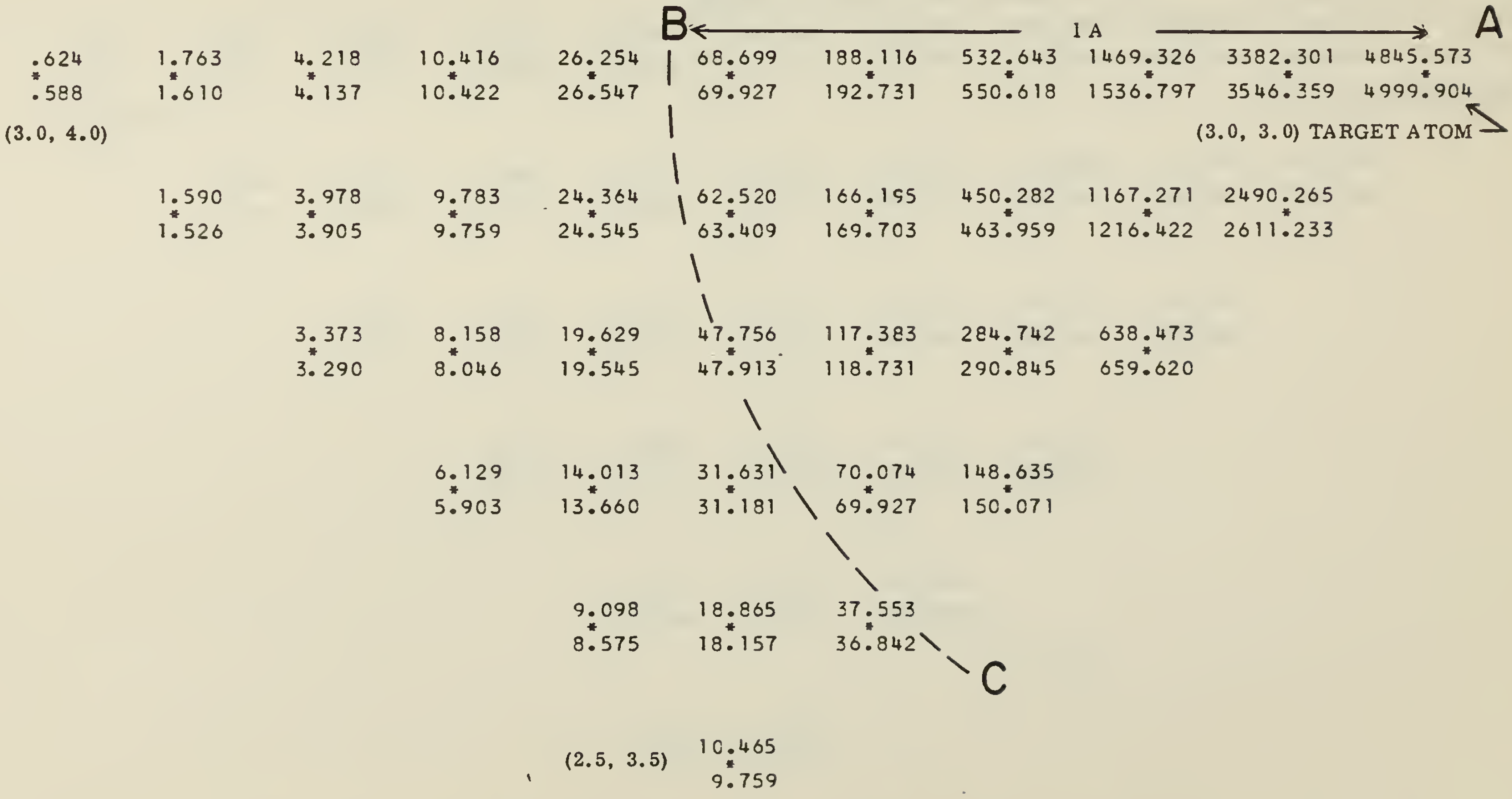
```
                         BORN-MAYER ERODED POTENTIAL        COPPER LATTICE AND BULLET
BULLET INCOMING ENERGY =  40.0  EV       TIME STEP MULTIPLIER = .C9C      BULLET INCIDENT ON (1CC) FACE

                            TOP NO. IS KINETIC ENERGY IN EV CF BULLET IN LATTICE
                        BOTTOM NC. IS KINETIC ENERGY IN EV CF BULLET IN TWOBODY PRCBLEM

                                                      E                                              A
  .062     3.689    16.151    23.567    21.358    17.3C8    12.517     7.702     3.648      .953      .011
    *        *        *         *         *         *         *          *         *         *         *
 39.334   37.954    35.222    31.CC2    25.578    19.5C6    13.433     7.983     3.686      .942      .CCC
(3.0, 4.0)                                                                       (3.0, 3.0) TARGET ATOM

           4.254    16.473    23.014    20.372    16.436    12.365     8.180     4.395     1.855
             *        *         *         *         *         *          *         *         *
          38.063    35.437    31.347    26.C6C    2C.118    14.159     8.8C1     4.573     1.871

                    12.378    19.893    17.785    13.861    11.529     8.666     6.454
                      *         *         *         *         *          *         *
                    36.C36    32.324    27.44C    21.881    16.259    11.177     7.151

                              16.159    14.C96     9.6C2     7.842     9.119
                                *         *         *         *          *
                              33.77C    29.522    24.580    19.5C6    14.872

                                        1C.196     6.979     5.566          F
                                          *         *         *
                                        32.CC8    27.878    23.535

                                        (2.5, 3.5)  5.926
                                                      *
                                                   31.347
```

Fig. 18. OUTPUT TRIANGLE for 40 ev bullet; (*) indicates impact point

```
                     BORN-MAYER ERODED POTENTIAL        COPPER LATTICE AND BULLET
        BULLET INCOMING ENERGY =  25.0   EV      TIME STEP MULTIPLIER = .C9C      BULLET INCIDENT ON (100) FACE

                            TOP NO. IS KINETIC ENERGY IN EV OF BULLET IN LATTICE
                          BOTTOM NC. IS KINETIC ENERGY IN EV OF 8ULLET IN TWOBODY PRCBLEM

                                                           E                                          A
   .195     3.755    12.597    12.848    12.014     9.442     6.848     4.212     1.989      .519      .011
     *        *         *         *         *         *         *         *         *         *         *
 24.251    23.012    20.905    18.001    14.559    10.918     7.418     4.363     2.000      .509      .CCC
(3.0, 4.0)                                                                           (3.0, 3.0) TARGET ATOM

            4.2C4    10.524    12.407    10.811     8.837     6.731     4.370     2.394     1.012
              *         *         *         *         *         *         *         *         *
           23.103    21.061    18.229    14.856    11.277     7.830     4.818     2.485     1.C12

                     10.439    11.146     8.960     7.096     6.174     4.703     3.517
                        *         *         *         *         *         *         *
                     21.504    18.882    15.715    12.321     9.032     6.145     3.903

                                8.816     6.478     4.198     3.811     4.888
                                  *         *         *         *         *
                               19.872    17.038    13.948    10.918     8.237

                                          4.108     2.382     2.016          F
                                            *         *         *
                                         18.669    15.990    13.314

                                        (2.5,3.5)   1.679
                                                      *
                                                   18.229
```

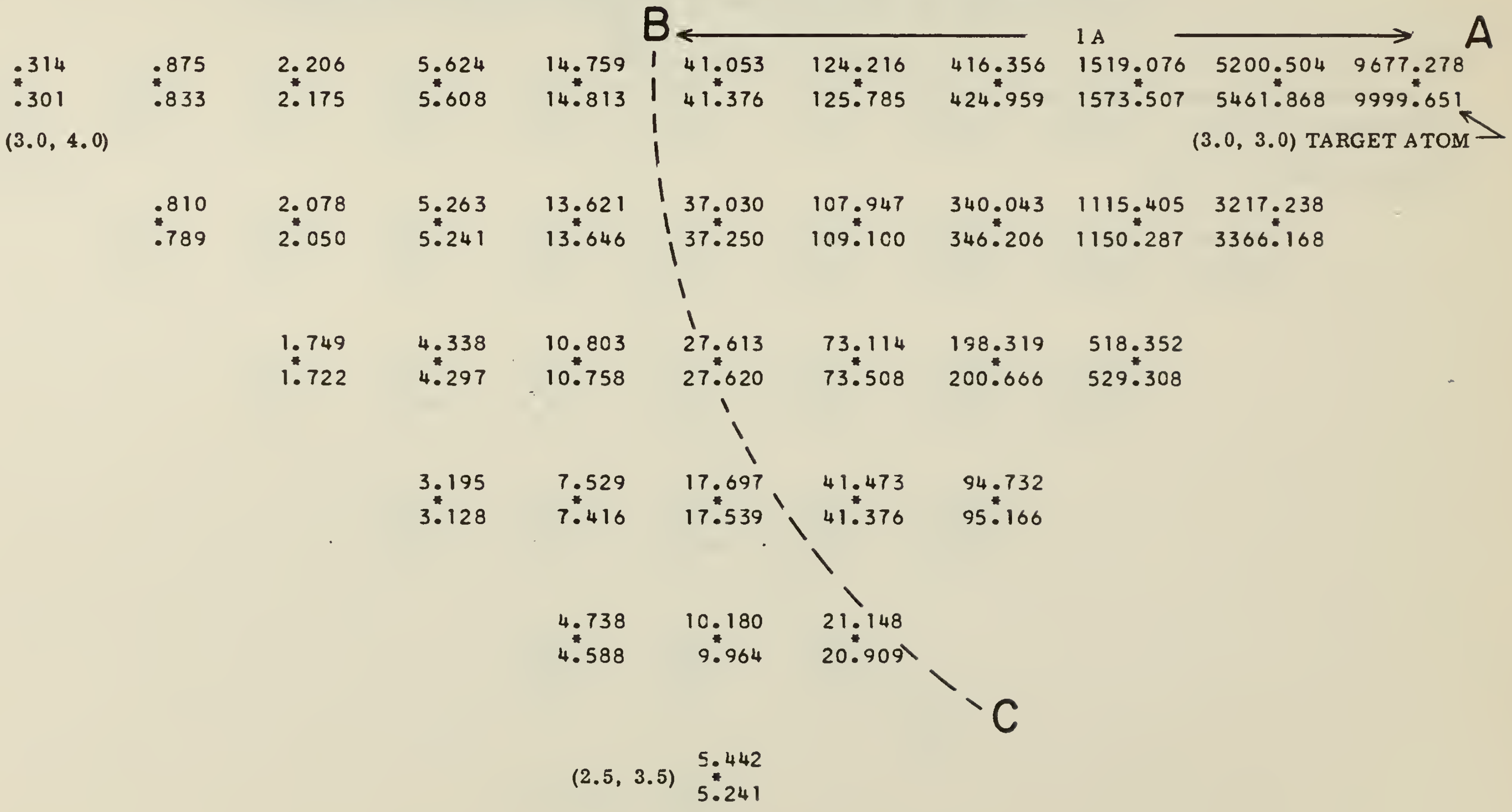
Fig. 19. OUTPUT TRIANGLE for 25 ev bullet; (*) indicates impact point

```
                 THOMAS-FERMI-FIRSOV POTENTIAL, ERODED, COPPER-COPPER
BULLET INCOMING ENERGY =5000.0  EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                     TOP NO. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE
                  BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN TWO BODY PROBLEM
```



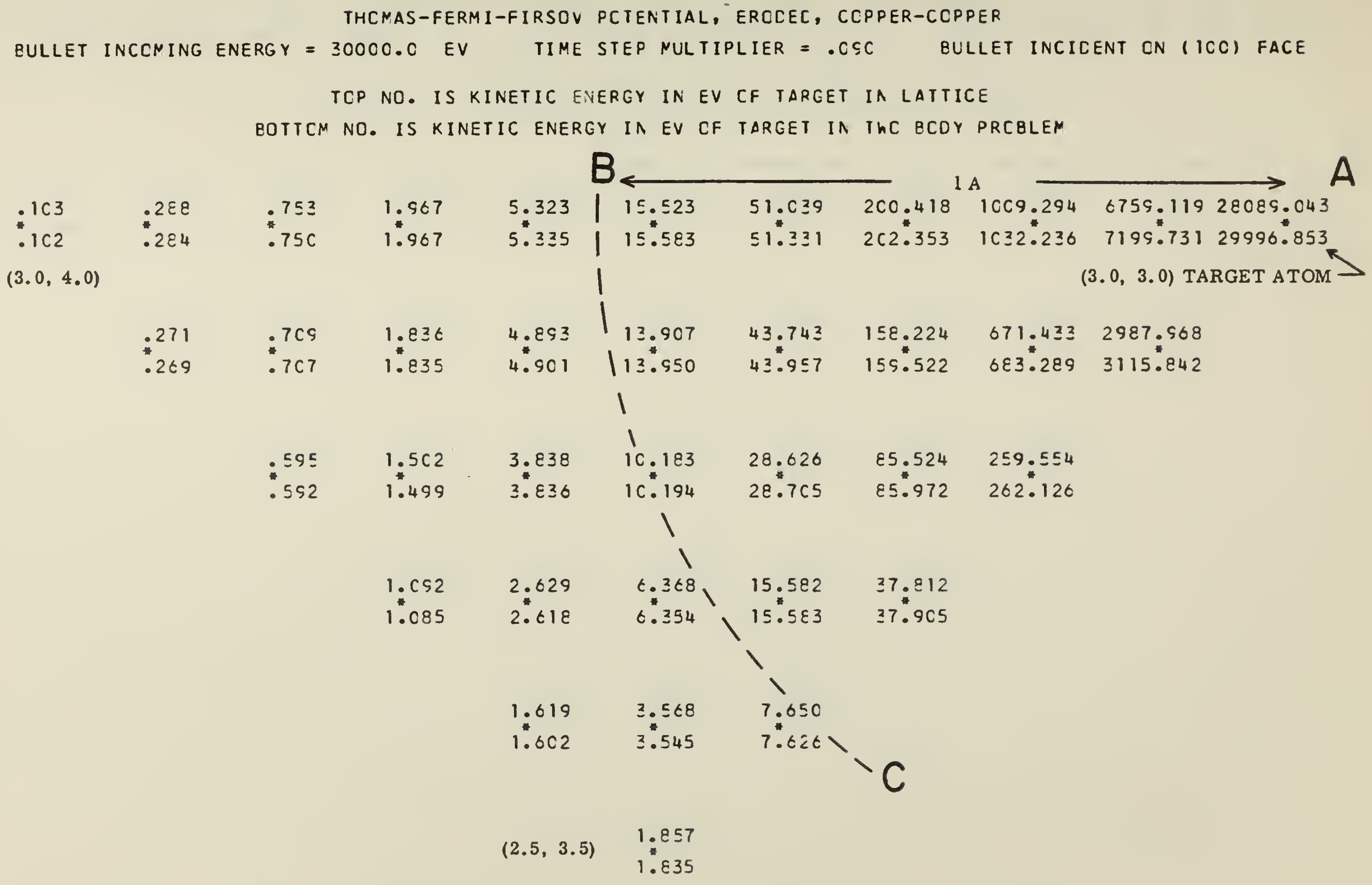
```
 .624     1.763     4.218    10.416    26.254    68.699   188.116   532.643  1469.326  3382.301  4845.573
  *         *         *         *         *         *         *         *         *         *         *
 .588     1.610     4.137    10.422    26.547    69.927   192.731   550.618  1536.797  3546.359  4999.904
(3.0, 4.0)                                                                   (3.0, 3.0) TARGET ATOM

          1.590     3.978     9.783    24.364    62.520   166.195   450.282  1167.271  2490.265
            *         *         *         *         *         *         *         *         *
          1.526     3.905     9.759    24.545    63.409   169.703   463.959  1216.422  2611.233

                    3.373     8.158    19.629    47.756   117.383   284.742   638.473
                      *         *         *         *         *         *         *
                    3.290     8.046    19.545    47.913   118.731   290.845   659.620

                              6.129    14.013    31.631    70.074   148.635
                                *         *         *         *         *
                              5.903    13.660    31.181    69.927   150.071

                                        9.098    18.865    37.553
                                          *         *         *
                                        8.575    18.157    36.842

                                   (2.5, 3.5)    10.465
                                                    *
                                                  9.759
```

Fig. 20. OUTPUT TRIANGLES for 5 kev bullet; (*) indicates impact point



```
                THOMAS-FERMI-FIRSOV POTENTIAL, ERODED, CCPPER-COPPER
BULLET INCOMING ENERGY = 10000   EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                TOP NO. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE
             BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN TWO BODY PROBLEM

                                                 B <--------------  1 A  ---------------> A
.314      .875      2.206     5.624     14.759    41.053    124.216   416.356   1519.076  5200.504  9677.278
*         *         *         *         *         *         *         *         *         *         *
.301      .833      2.175     5.608     14.813    41.376    125.785   424.959   1573.507  5461.868  9999.651
(3.0, 4.0)                                                                      (3.0, 3.0) TARGET ATOM

          .810      2.078     5.263     13.621    37.030    107.947   340.043   1115.405  3217.238
          *         *         *         *         *         *         *         *         *
          .789      2.050     5.241     13.646    37.250    109.100   346.206   1150.287  3366.168

                    1.749     4.338     10.803    27.613    73.114    198.319   518.352
                    *         *         *         *         *         *         *
                    1.722     4.297     10.758    27.620    73.508    200.666   529.308

                              3.195     7.529     17.697    41.473    94.732
                              *         *         *         *         *
                              3.128     7.416     17.539    41.376    95.166

                                        4.738     10.180    21.148
                                        *         *         *
                                        4.588     9.964     20.909
                                                                      C

                                     (2.5, 3.5) 5.442
                                                *
                                                5.241
```

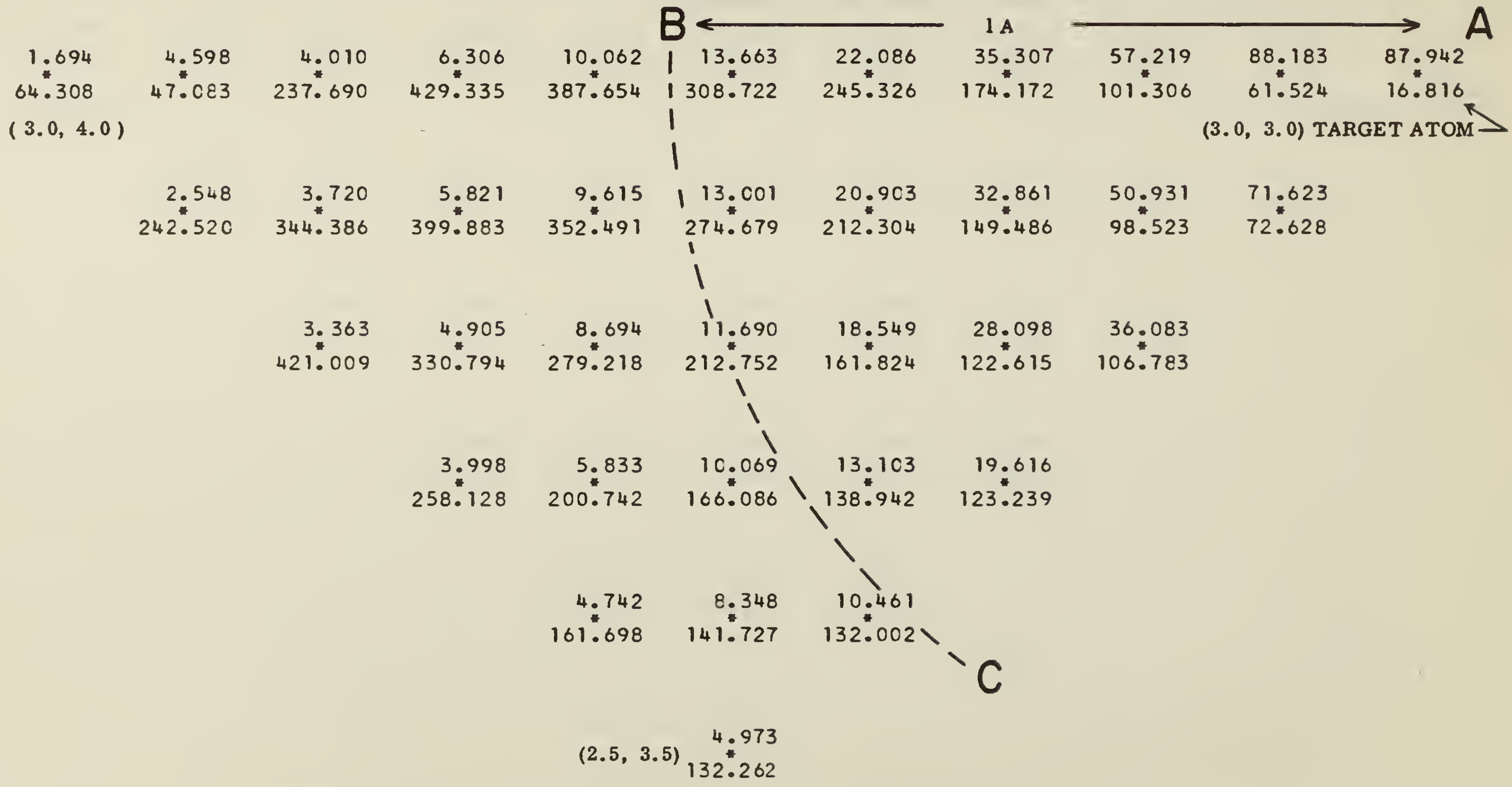
Fig. 21. OUTPUT TRIANGLE for 10 kev bullet; (*) indicates impact point



```
                        THOMAS-FERMI-FIRSOV POTENTIAL, ERODED, COPPER-COPPER
   BULLET INCOMING ENERGY = 30000.0  EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                        TOP NO. IS KINETIC ENERGY IN EV OF TARGET IN LATTICE
                     BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN TWO BODY PROBLEM

                                                      B                  1 A                   A
 .103     .288     .753     1.967     5.323     15.523    51.039    200.418   1009.294   6759.119  28089.043
   *        *        *        *         *          *         *          *         *          *          *
 .102     .284     .750     1.967     5.335     15.583    51.331    202.353   1032.236   7199.731  29996.853

(3.0, 4.0)                                                                       (3.0, 3.0) TARGET ATOM

          .271     .709     1.836     4.893     13.907    43.743    158.224    671.433   2987.968
            *        *        *         *          *         *          *         *          *
          .269     .707     1.835     4.901     13.950    43.957    159.522    683.289   3115.842

                   .595     1.502     3.838     10.183    28.626     85.524    259.554
                     *        *         *          *         *          *         *
                   .592     1.499     3.836     10.194    28.705     85.972    262.126

                            1.092     2.629      6.368    15.582     37.812
                              *         *          *         *          *
                            1.085     2.618      6.354    15.583     37.905

                                      1.619      3.568     7.650
                                        *          *         *
                                      1.602      3.545     7.626
                                                                 C

                                   (2.5, 3.5)    1.857
                                                   *
                                                 1.835
```

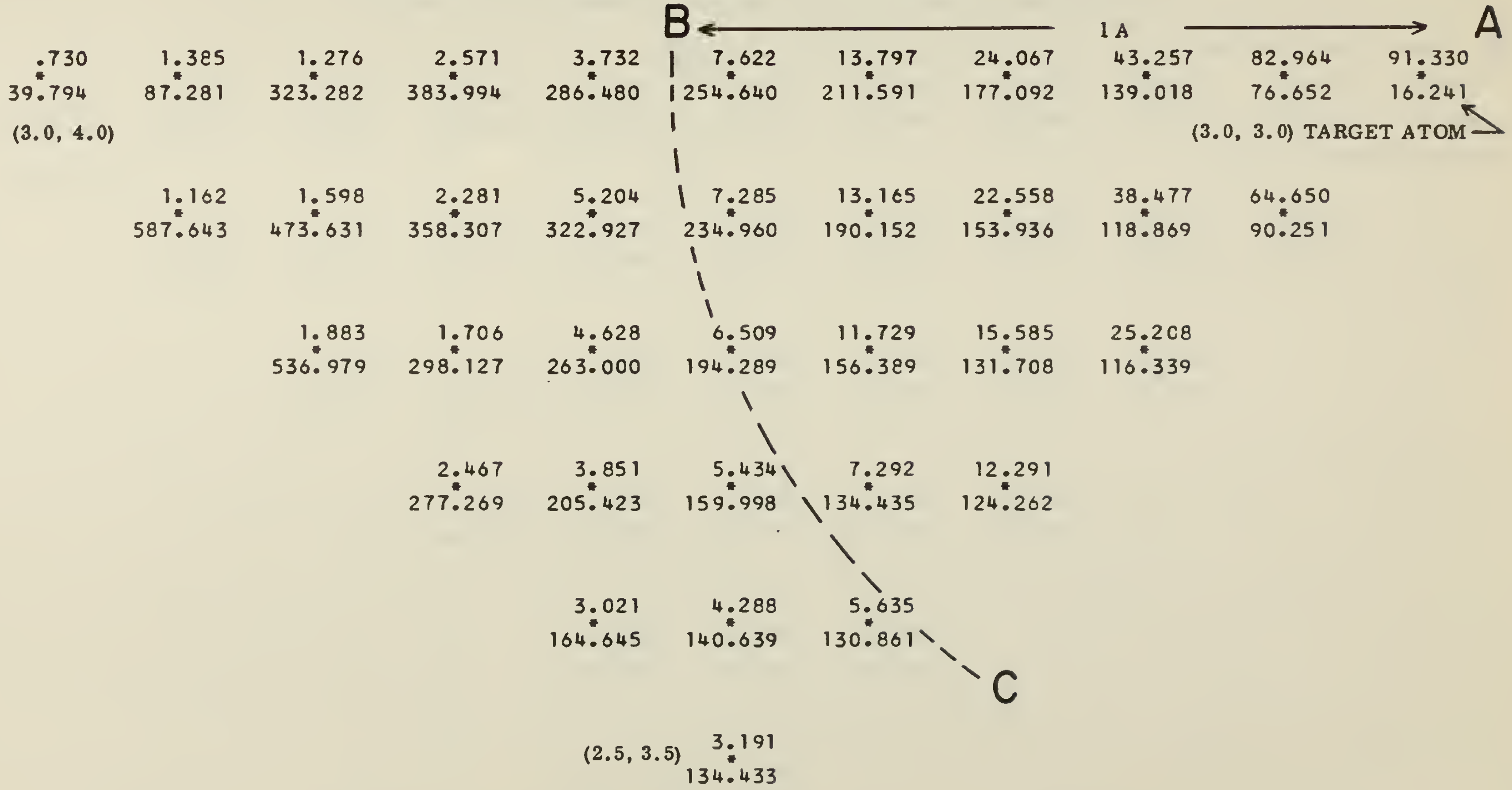
Fig. 22. OUTPUT TRIANGLE for 30 kev bullet; (*) indicates impact point

```
                      THOMAS-FERMI-FIRSOV POTENTIAL, ERODED, COPPER-COPPER
BULLET INCOMING ENERGY =5000.0  EV      TIME STEP MULTIPLIER = .090      BULLET INCIDENT ON (100) FACE

                      TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LATTICE
                      BOTTOM NO. IS POTENTIAL ENERGY IN EV OF BULLET IN LATTICE
```



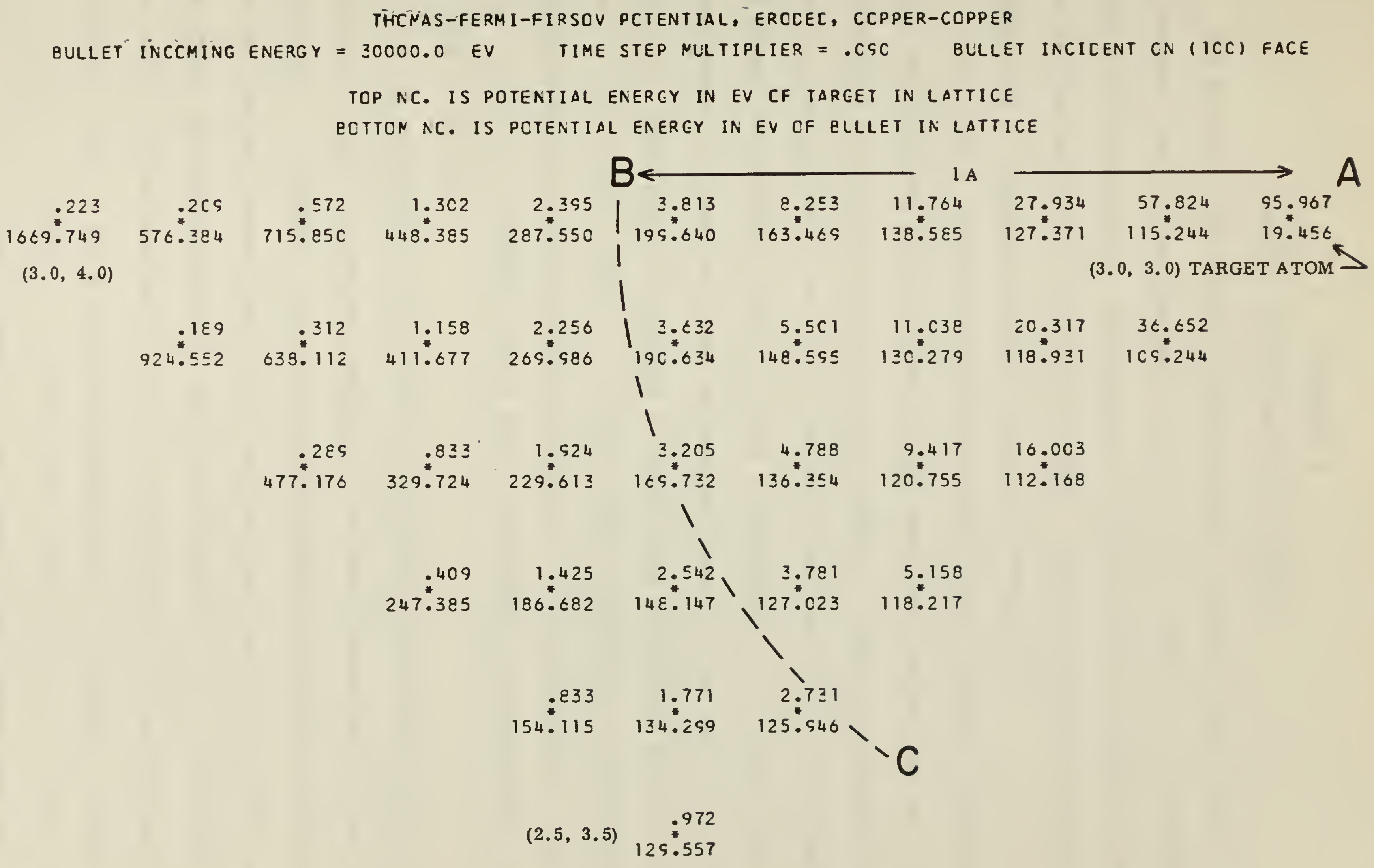
```
  1.694     4.598     4.010     6.306    10.062    13.663    22.086    35.307    57.219    88.183    87.942
    *         *         *         *         *         *         *         *         *         *         *
 64.308    47.083   237.690   429.335   387.654   308.722   245.326   174.172   101.306    61.524    16.816
( 3.0, 4.0 )                                                                          (3.0, 3.0) TARGET ATOM

            2.548     3.720     5.821     9.615    13.001    20.903    32.861    50.931    71.623
              *         *         *         *         *         *         *         *         *
          242.520   344.386   399.883   352.491   274.679   212.304   149.486    98.523    72.628

                      3.363     4.905     8.694    11.690    18.549    28.098    36.083
                        *         *         *         *         *         *         *
                    421.009   330.794   279.218   212.752   161.824   122.615   106.783

                                3.998     5.833    10.069    13.103    19.616
                                  *         *         *         *         *
                                258.128   200.742   166.086   138.942   123.239

                                          4.742     8.348    10.461
                                            *         *         *
                                          161.698   141.727   132.002

                                        (2.5, 3.5)  4.973
                                                      *
                                                    132.262
```

Fig. 23. OUTPUT TRIANGLE for 5 kev bullet; (*) indicates impact point



```
                 THOMAS-FERMI-FIRSOV POTENTIAL, ERODED, COPPER-COPPER
BULLET INCOMING ENERGY = 10000   EV     TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                 TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LATTICE
                 BOTTOM NO. IS POTENTIAL ENERGY IN EV OF BULLET IN LATTICE

   .730     1.385     1.276     2.571     3.732     7.622    13.797    24.067    43.257    82.964    91.330
     *        *         *         *         *         *         *         *         *         *         *
 39.794    87.281   323.282   383.994   286.480   254.640   211.591   177.092   139.018    76.652    16.241
(3.0, 4.0)                                                                   (3.0, 3.0) TARGET ATOM

            1.162     1.598     2.281     5.204     7.285    13.165    22.558    38.477    64.650
              *         *         *         *         *         *         *         *         *
          587.643   473.631   358.307   322.927   234.960   190.152   153.936   118.869    90.251

                      1.883     1.706     4.628     6.509    11.729    15.585    25.208
                        *         *         *         *         *         *         *
                    536.979   298.127   263.000   194.289   156.389   131.708   116.339

                                2.467     3.851     5.434     7.292    12.291
                                  *         *         *         *         *
                              277.269   205.423   159.998   134.435   124.262

                                          3.021     4.288     5.635
                                            *         *         *
                                        164.645   140.639   130.861

                                     (2.5, 3.5) 3.191
                                                  *
                                               134.433
```

Fig. 24. OUTPUT TRIANGLE for 10 kev bullet; (*) indicates impact point



```
                              THOMAS-FERMI-FIRSOV POTENTIAL, ERODEC, COPPER-COPPER
        BULLET INCOMING ENERGY = 30000.0  EV      TIME STEP MULTIPLIER = .090     BULLET INCIDENT ON (100) FACE

                              TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LATTICE
                             BOTTOM NO. IS POTENTIAL ENERGY IN EV OF BULLET IN LATTICE

    .223      .209      .572     1.302     2.395     3.813     8.253    11.764    27.934    57.824    95.967
      *         *         *         *         *         *         *         *         *         *         *
1669.749   576.384   715.850   448.385   287.550   199.640   163.469   138.585   127.371   115.244    19.456

              .189      .312     1.158     2.256     3.632     5.501    11.038    20.317    36.652
                *         *         *         *         *         *         *         *         *
           924.552   638.112   411.677   269.986   190.634   148.595   130.279   118.931   109.244

                        .289      .833     1.924     3.205     4.788     9.417    16.003
                          *         *         *         *         *         *         *
                     477.176   329.724   229.613   169.732   136.354   120.755   112.168

                                  .409     1.425     2.542     3.781     5.158
                                    *         *         *         *         *
                               247.385   186.682   148.147   127.023   118.217

                                            .833     1.771     2.731
                                              *         *         *
                                         154.115   134.299   125.946

                                                      .972
                                                        *
                                                   129.557
```

Fig. 25. OUTPUT TRIANGLE for 30 KEV bullet; (*) indicates impact point

APPENDIX I

GENERAL DISCUSSION OF THE PROGRAM

The masses of the lattice atoms are equal to that of copper and are an integral part of the program. The bullet mass however, can be varied by changing the input data. The potentials and forces are calculated by function subroutines at the end of the program. The main program is not disrupted when a different potential function is substituted.

A coordinate system was established with an atom located at the origin. For a face centered cubic lattice in this coordinate system, the sum of the coordinates of an atom is always an even number. Fixed point numbers were used for lattice units, and the volume which contains all the atoms (movable and fixed) was scanned in the x, y, and z directions. If the sum of the coordinates of a point was even, an atom was placed there, otherwise a space was left. Truncation of quotients in fixed point arithmetic allows a simple test for odd or even numbers. The fixed point coordinates of the atoms were stored in memory as floating point numbers for later calculations. The "core" atoms were assigned numbers from 2-64 and the fixed atoms were numbered from 65 to 172.

In the calculation of the forces or potentials associated with an atom, the atoms closer than nearest neighbors in an undisturbed lattice must be considered. A "nested" Do loop was used for these calculations. The outside Do loop was indexed from 1 to 64 and the inner Do loops initial index was always one greater than the outer Do and ended at 172. This arrangement avoids the calculation of forces or potentials twice for the same pair of atoms. The x, y and z coordinate separations, in that order, between the atom under consideration (index of outer loop) and any other atom were tested. If any of these separations were found to be greater than ROE,

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

the inner Do index was advanced by one. If the coordinates passed these three tests, the square of the distance between atoms was compared to the square of ROE (ROE2). The true distance of any atom that passed this test was used in the force or potential function and the result applied to both atoms. (In potential calculations, half the potential was given to each atom). If the square of the distance between atoms was equal to or greater than ROE2, the inner Do index was advanced by one. Most of the atoms will be eliminated in the first three tests. The procedure avoids time consuming square root calculations by the computer.

The double iteration method used to move atoms requires two calculations of resultant forces for each "time step". The same section of the program was used for both force calculations, but the equations required to move the atoms twice in the time step are not identical. The fixed point variable INDEX was used as a switching device to jump over the motion equations that locate the atoms at temporary positions. The jump is executed after the second calculation of forces.

The movement of atoms is continued until the kinetic energy of the target is a maximum. It is necessary to advance one time step beyond the maximum to establish the maximum. The particle locations and velocities at the time of the maximum are still in memory, and these are used in kinetic and potential energy calculations or as output.

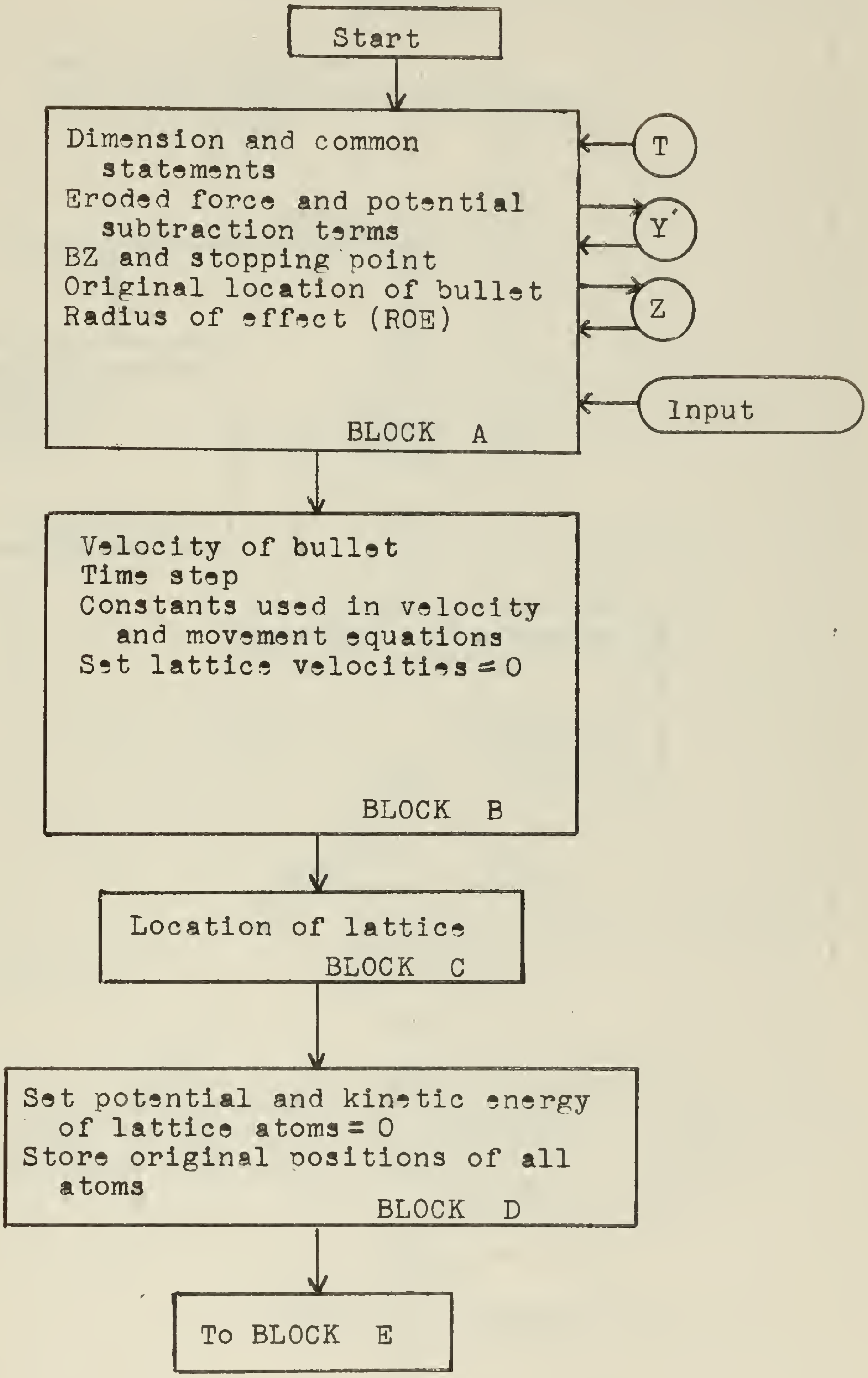
Although the two body problem is in two dimensions, the impact parameter is the same as that in the lattice. The two body problem is solved in the same manner as the lattice except that the interaction is stopped when the atoms are separated by a distance equal to ROE which means the potential and force between atoms is zero. The interaction is initially started with the separation of atoms slightly less than ROE. The ΔT for

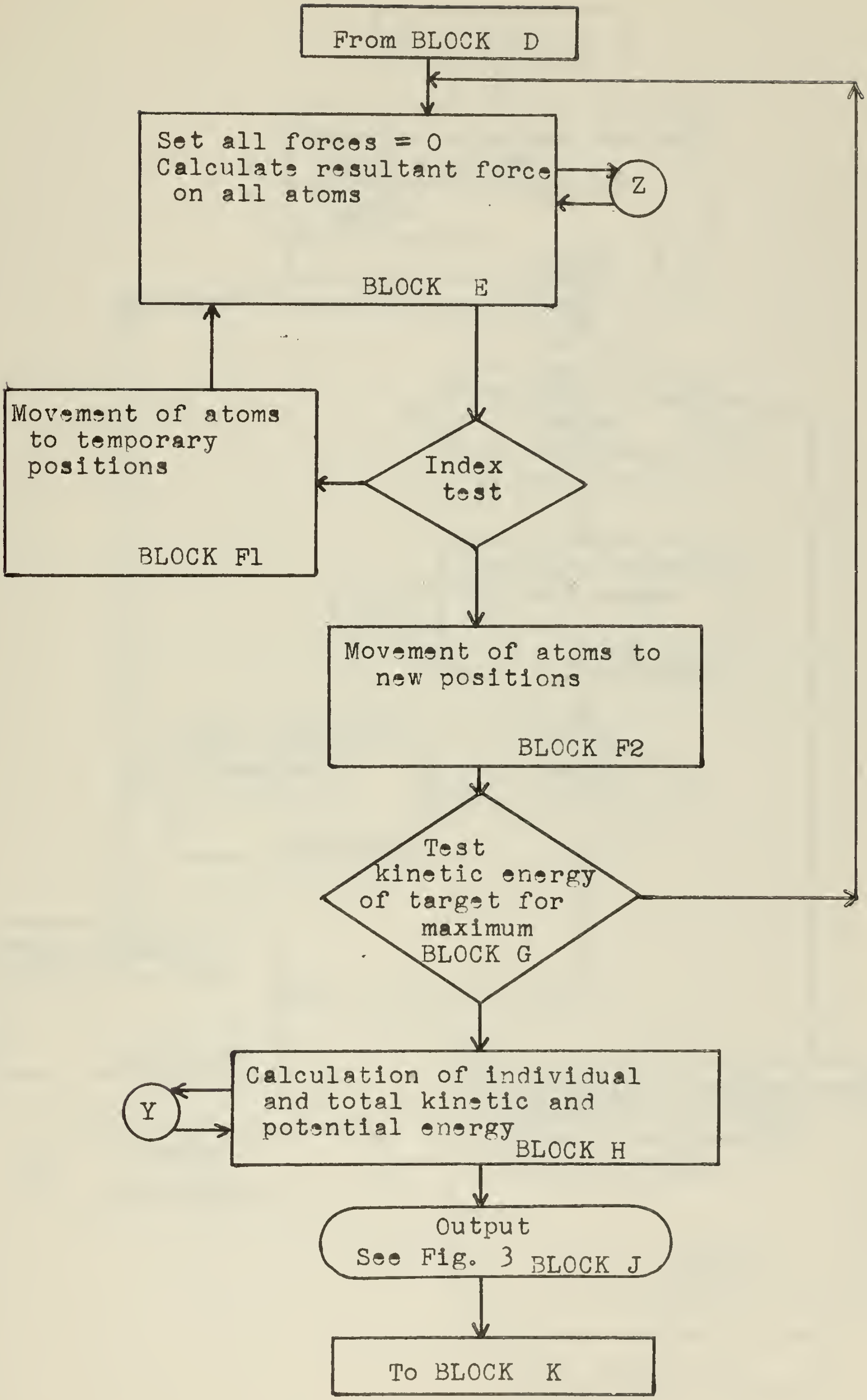
the two body problem is much smaller than the one used for lattice calculations. The small ΔT consistantly produces very much more accurate results in the two body problem than in the lattice.

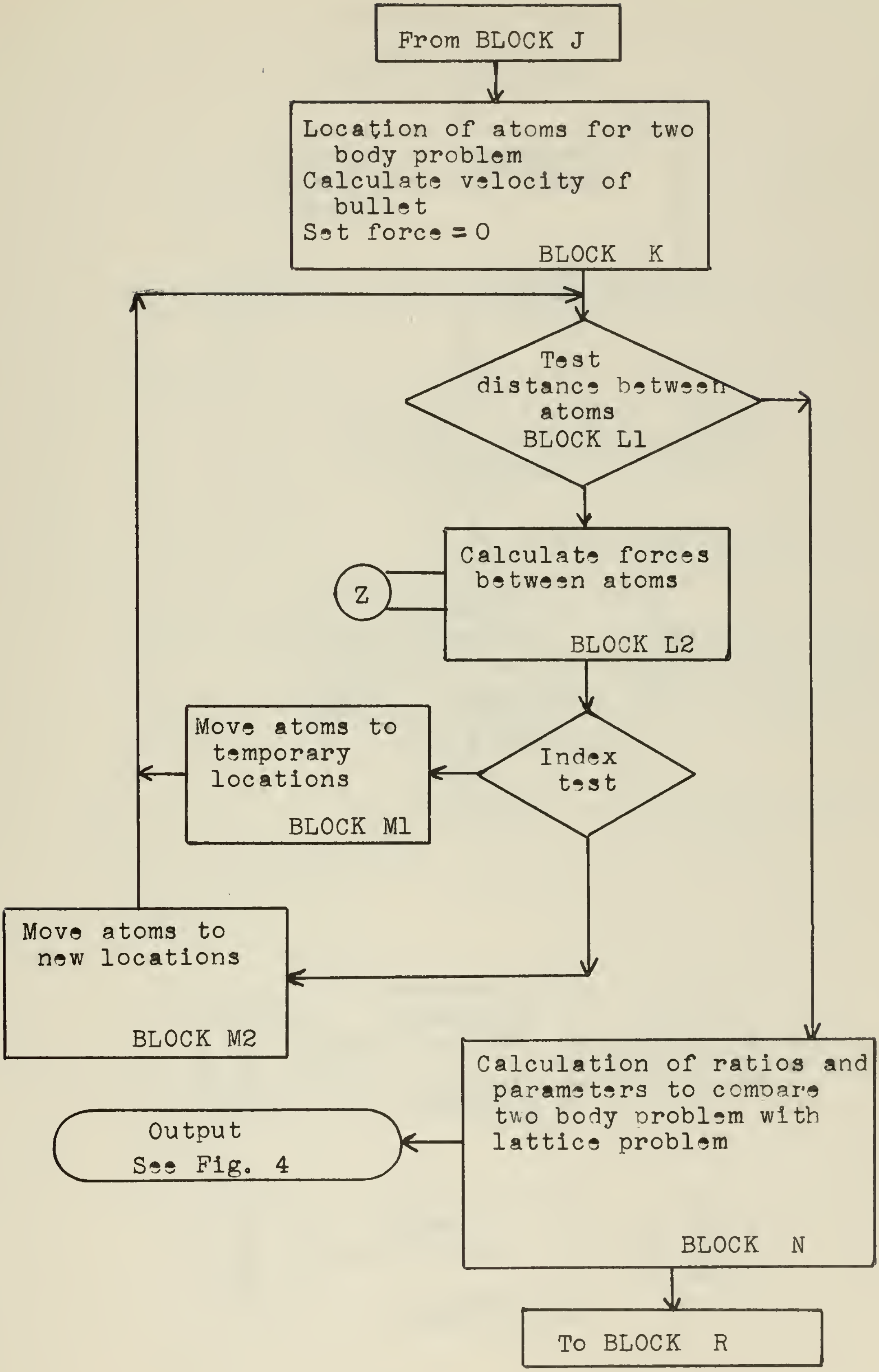
The input consists of the bullet energy and mass, its x coordinate, and the time step multiplier. In order to calculate data for all 36 impact points, six input cards are required; each is identical except for the x coordinate of the bullet. The x coordinates assigned are 3.0, 2.9, 2.8, 2.7, 2.6, and 2.5 in that order. After receiving the input from one card, the corresponding z coordinate on the line AB is calculated (see Fig. 6). The computer proceeds through the program for this point, then subtracts 0.1 lattice units from the z coordinate and repeats. It procedes down a column until all calculations for impact points on the line BC have been made. The computer pauses at this point to await instructions. Here it may receive a new data card and start another column. After the calculations for the point on the apex of the triangle ($x=2.5$, $z=3.5$) are complete, the computer can be directed to print the output in the triangular form shown by Fig. 6.

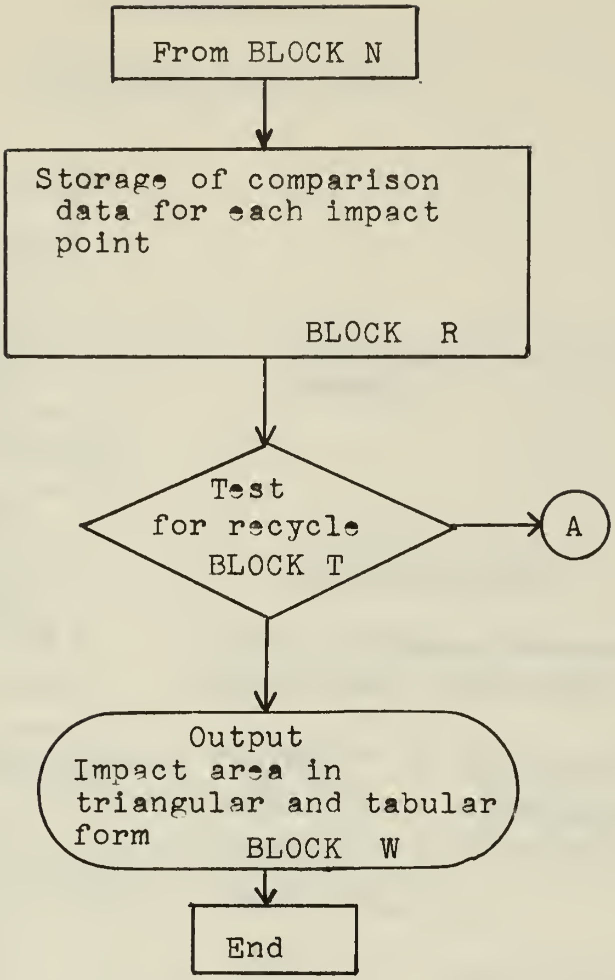
APPENDIX II

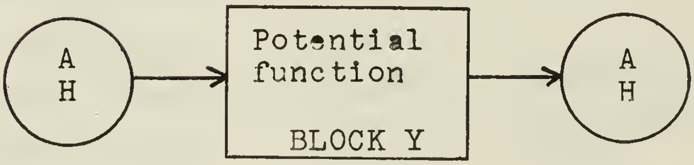
BLOCK DIAGRAM

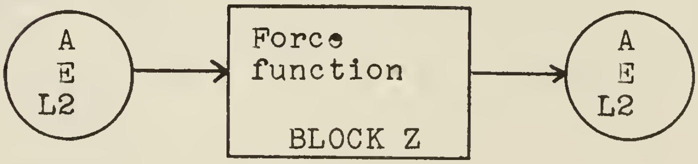

Start
Dimension and common statements
Eroded force and potential subtraction terms
BZ and stopping point
Original location of bullet
Radius of effect (ROE)
BLOCK A
T
Y′
Z
Input
Velocity of bullet
Time step
Constants used in velocity and movement equations
Set lattice velocities = 0
BLOCK B
Location of lattice
BLOCK C
Set potential and kinetic energy of lattice atoms = 0
Store original positions of all atoms
BLOCK D
To BLOCK E


From BLOCK D
Set all forces = 0
Calculate resultant force on all atoms
BLOCK E
Z
Movement of atoms to temporary positions
BLOCK F1
Index test
Movement of atoms to new positions
BLOCK F2
Test kinetic energy of target for maximum
BLOCK G
Calculation of individual and total kinetic and potential energy
BLOCK H
Y
Output
See Fig. 3
BLOCK J
To BLOCK K


From BLOCK J
Location of atoms for two body problem
Calculate velocity of bullet
Set force = 0
BLOCK K
Test distance between atoms
BLOCK L1
Calculate forces between atoms
BLOCK L2
Z
Index test
Move atoms to temporary locations
BLOCK M1
Move atoms to new locations
BLOCK M2
Calculation of ratios and parameters to compare two body problem with lattice problem
BLOCK N
Output
See Fig. 4
To BLOCK R


From BLOCK N
Storage of comparison data for each impact point
BLOCK R
Test for recycle
BLOCK T
A
Output
Impact area in triangular and tabular form
BLOCK W
End

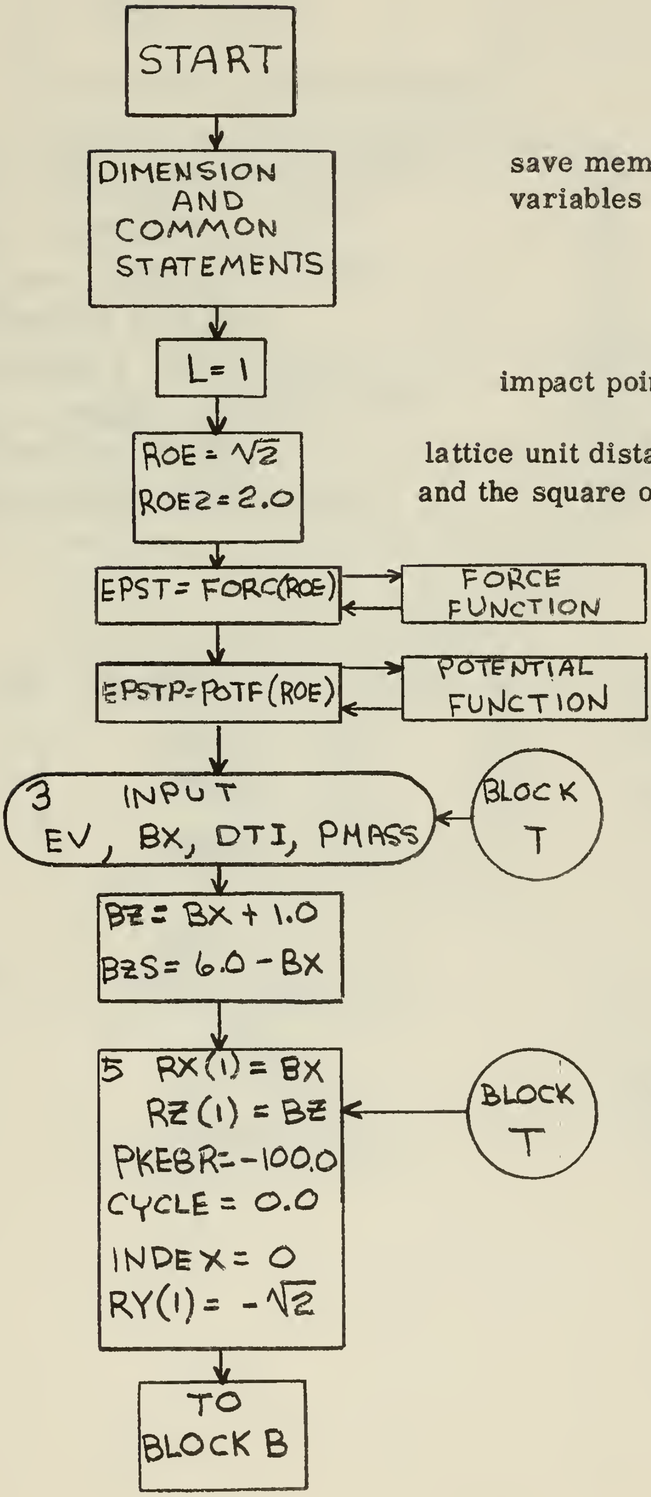

A
H
Potential function
BLOCK Y
A
H


A
E
L2
Force function
BLOCK Z
A
E
L2

APPENDIX III

DETAILED FLOW CHART

BLOCK A



save memory locations for subscripted variables

impact point number

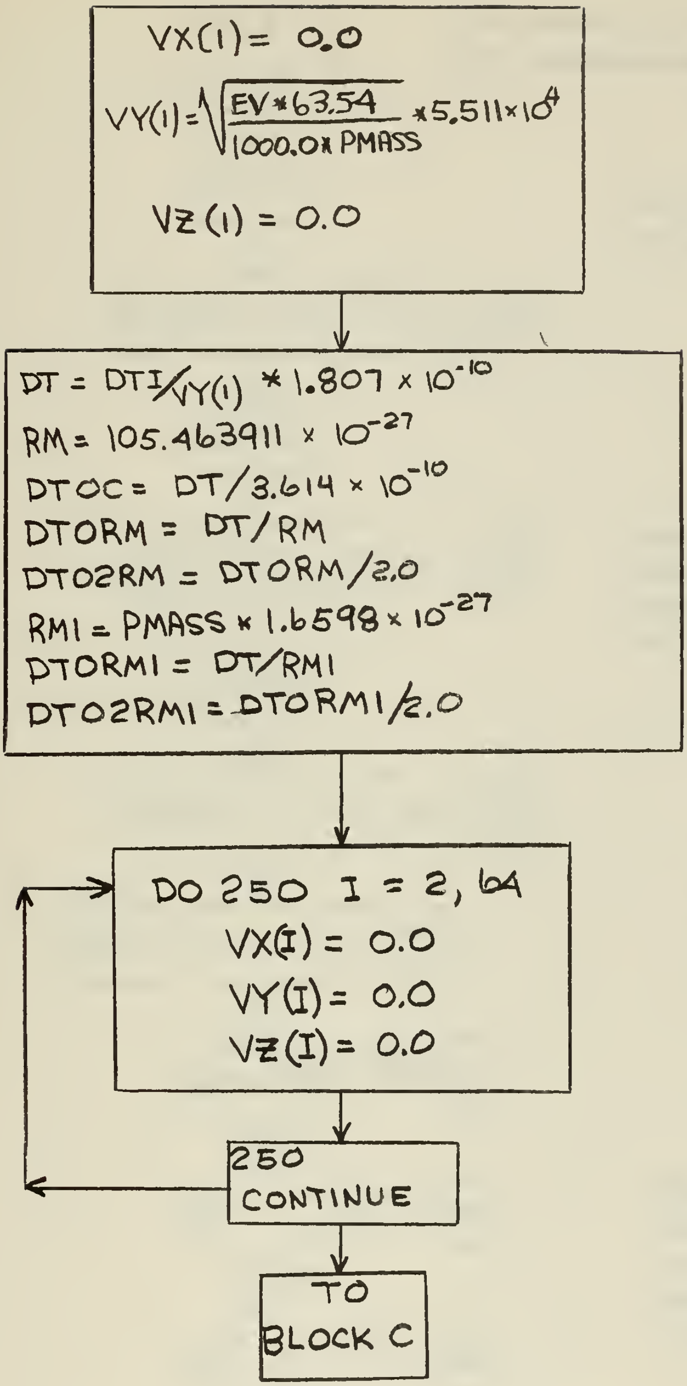
lattice unit distance between nearest neighbors and the square of that distance

terms subtracted from calculated potential and force that "erode" them

starts here for every "column" in impact area

starts here for every impact point; assigns coordinates to bullet

BLOCK B

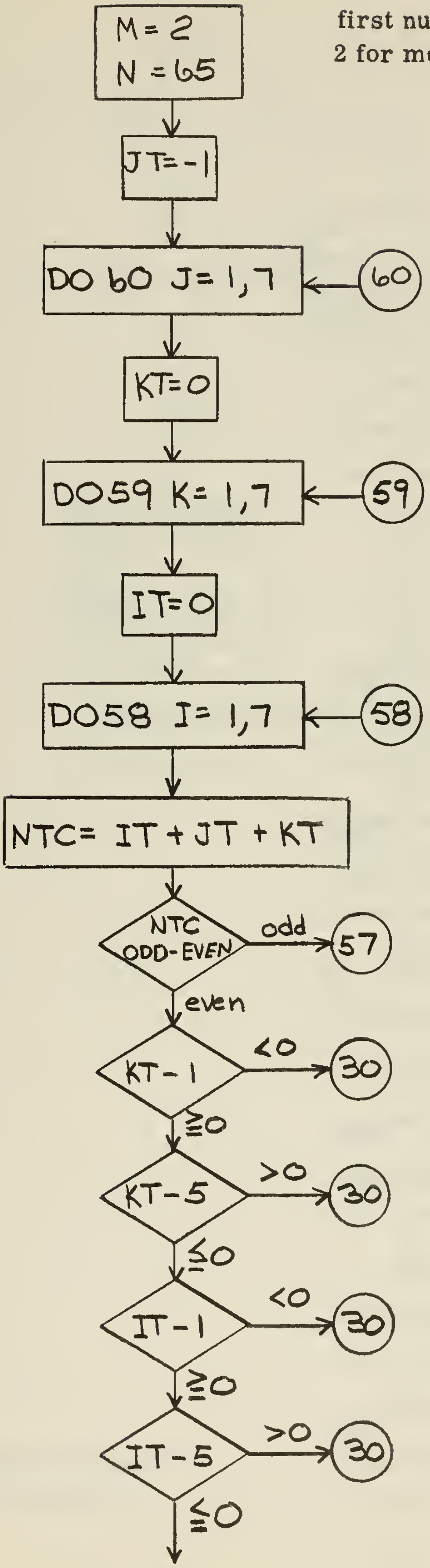


velocity components of bullet

calculates constants used in force and movement equations

sets velocity of lattice atoms to zero

BLOCK C



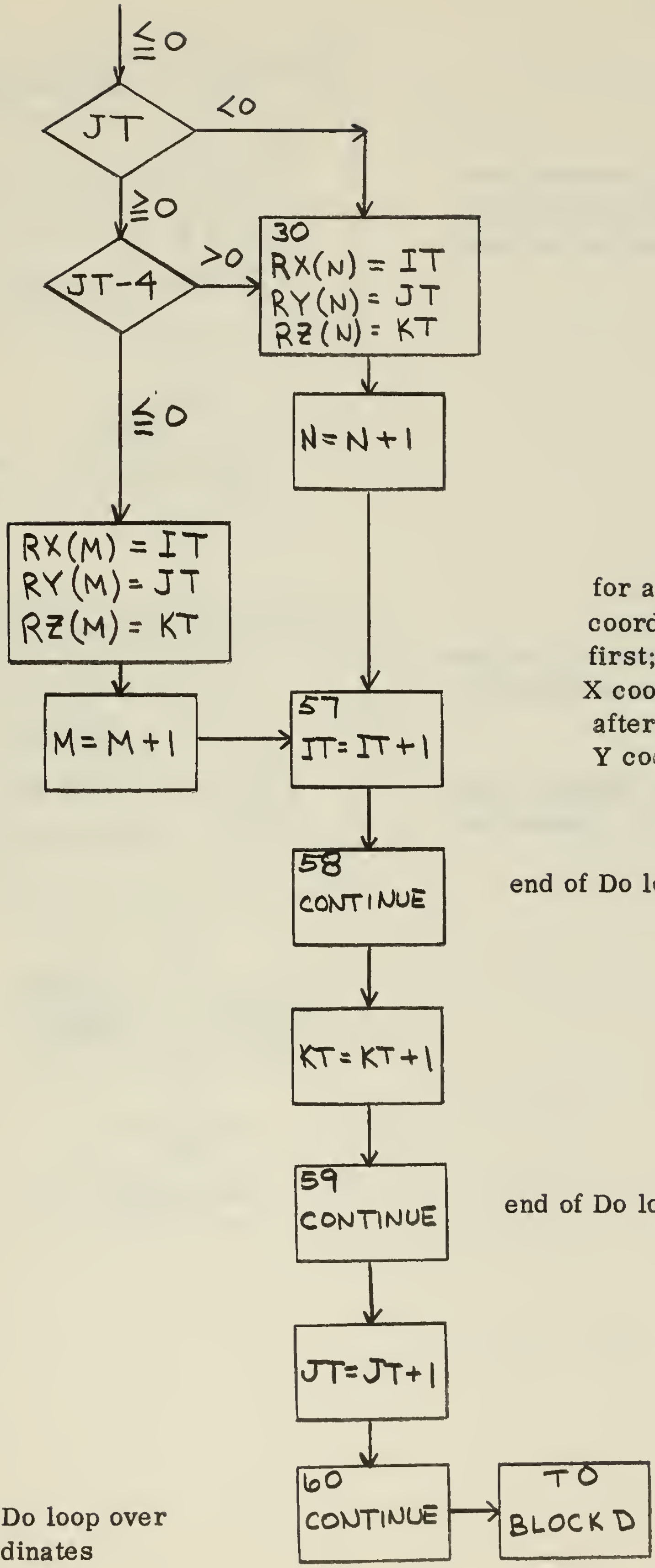
first numbers to be assigned to lattice atoms
2 for movable core, 65 for fixed atoms

IT, JT, KT are X, Y, Z coordinates in the system used for reference

each point with integer values for coordinates is tested; if the sum of the coordinates is an even number, an atom is assigned to that position

these decision processes determine if an atom is in the "core"; this is necessary in order to have core atoms with consecutive numbers 2-64

BLOCK C (con't)



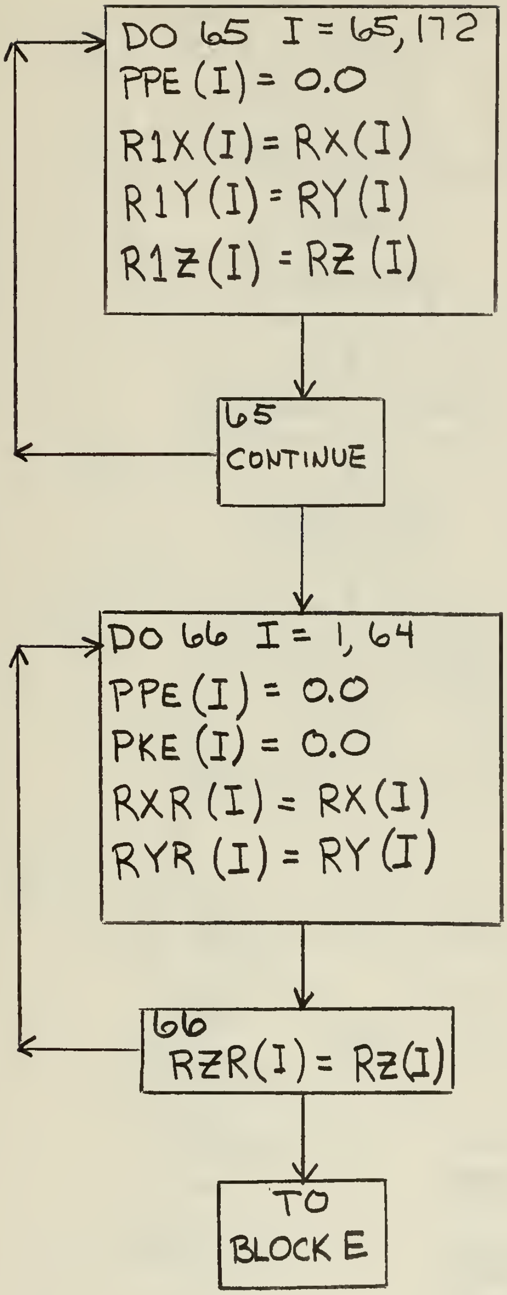
for a given Y and Z, X coordinates are checked first; then Z is changed and X coordinates checked again; after tests on X and Z , Y coordinate is changed

end of Do loop over X coordinates

end of Do loop over Z coordinates

end of Do loop over Y coordinates

BLOCK D

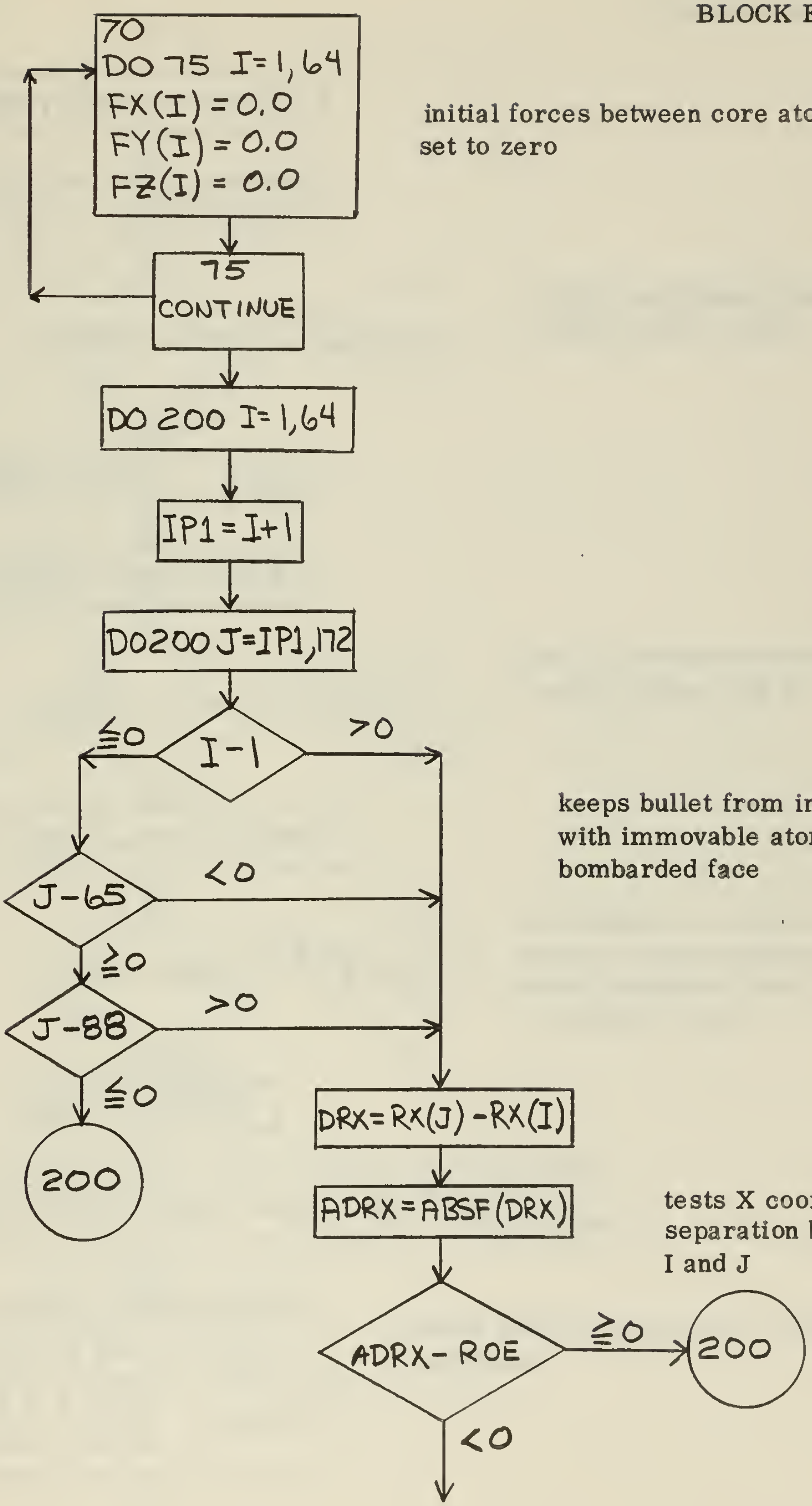


sets temporary and permanent coordinates of immovable atoms equal to eachother

sets initial potential and kinetic energy of core atoms equal to zero

stores original positions of bullet and core atoms

BLOCK E

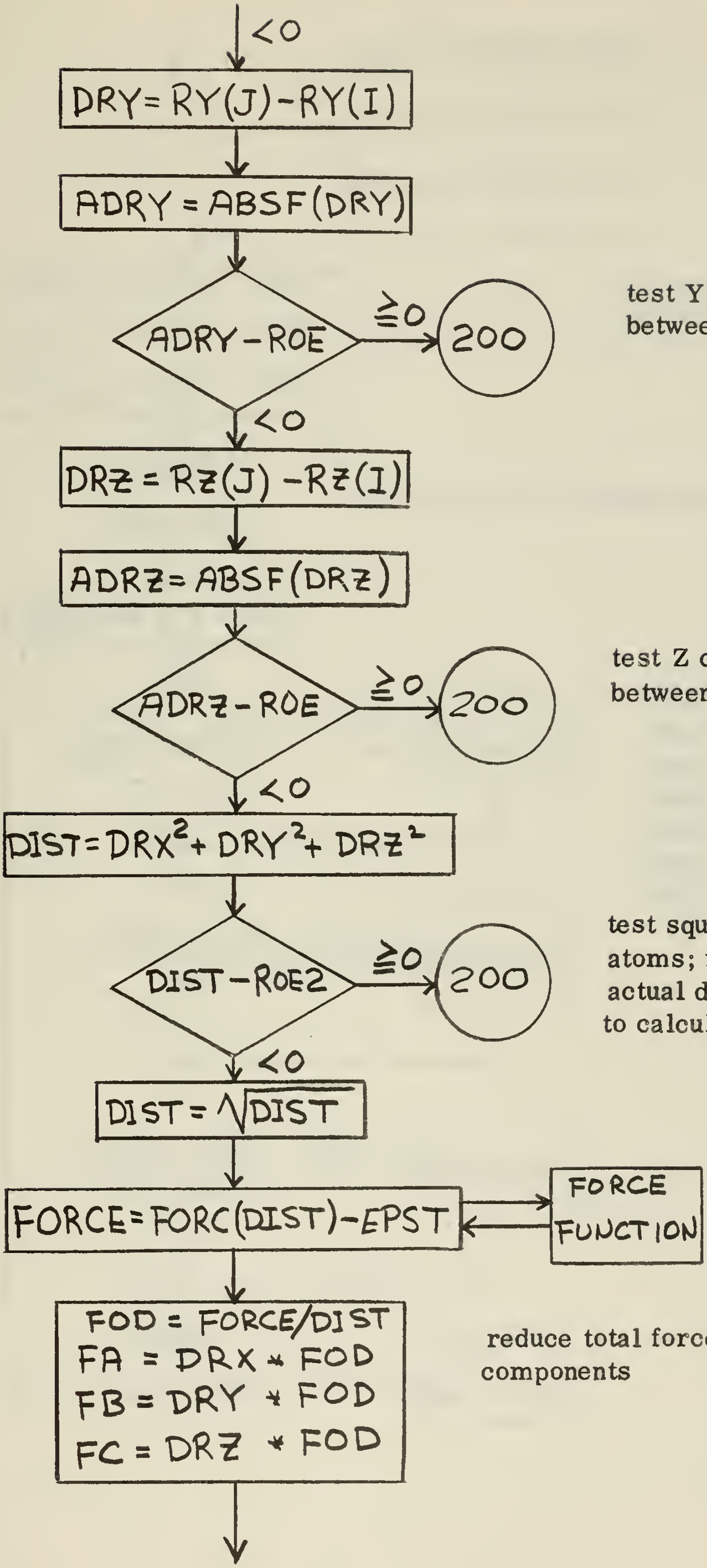


initial forces between core atoms set to zero

keeps bullet from interacting with immovable atoms covering bombarded face

tests X coordinate separation between atom I and J

BLOCK E (con't)



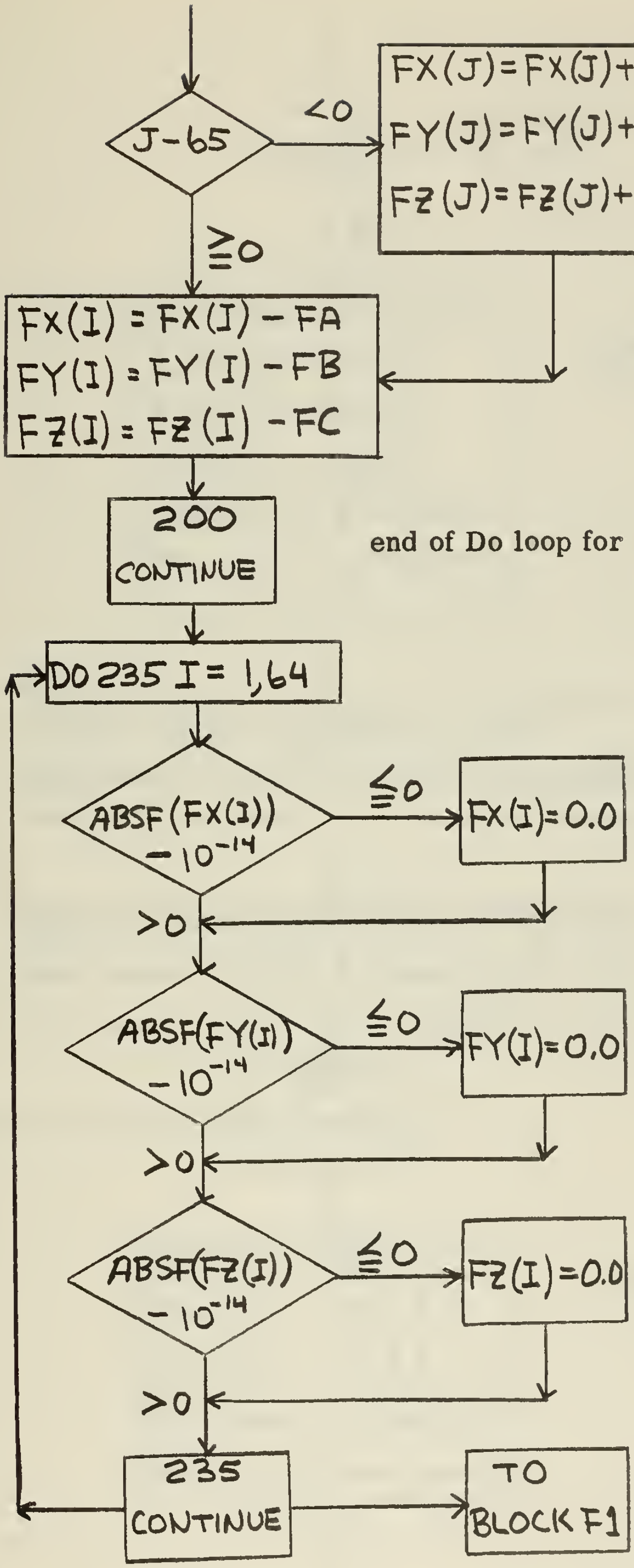
test Y coordinate separation between atom I and J

test Z coordinate separation between atom I and J

test square of distance between atoms; if square passes test, actual distance is found and used to calculate force

reduce total force into X, Y, and Z components

BLOCK E (con't)

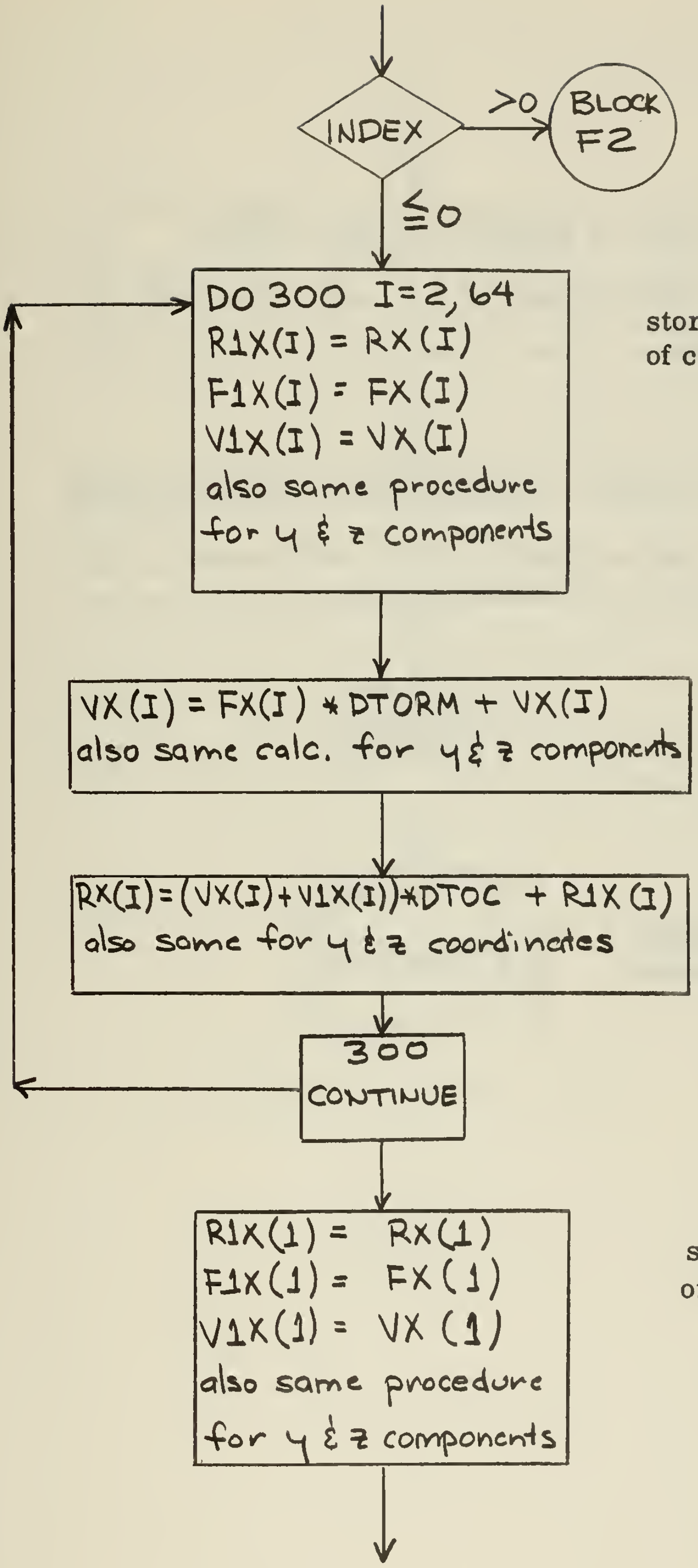


add force to total forces on atoms I and J if they are in the core

end of Do loop for finding forces

round off procedures in computer may lead to very small resultant forces in situations where the forces should be zero; this procedure sets to zero any resultant force less than 10^{-14} newtons

BLOCK F1


INDEX
>0
BLOCK F2
≦0
DO 300 I=2, 64
R1X(I) = RX(I)
F1X(I) = FX(I)
V1X(I) = VX(I)
also same procedure for y & z components
VX(I) = FX(I) * DTORM + VX(I)
also same calc. for y & z components
RX(I)=(VX(I)+V1X(I))*DTOC + R1X(I)
also same for y & z coordinates
300 CONTINUE
R1X(1) = RX(1)
F1X(1) = FX(1)
V1X(1) = VX(1)
also same procedure for y & z components

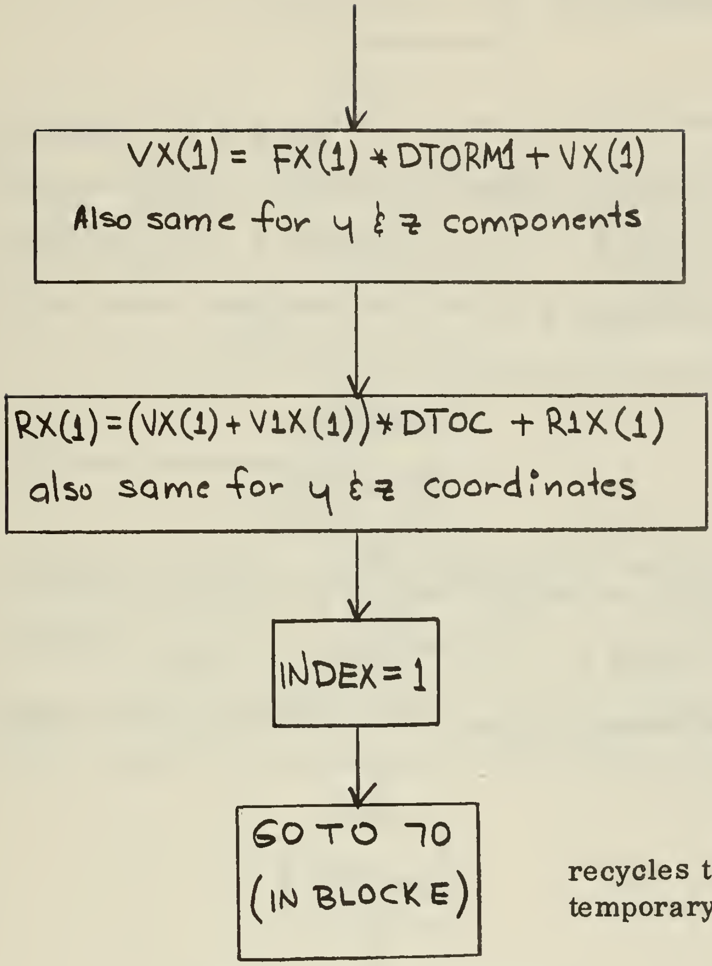
store position, velocity, and force of core atoms

calculate temporary velocities

move core atoms to temporary locations

store position, velocity, and force of bullet

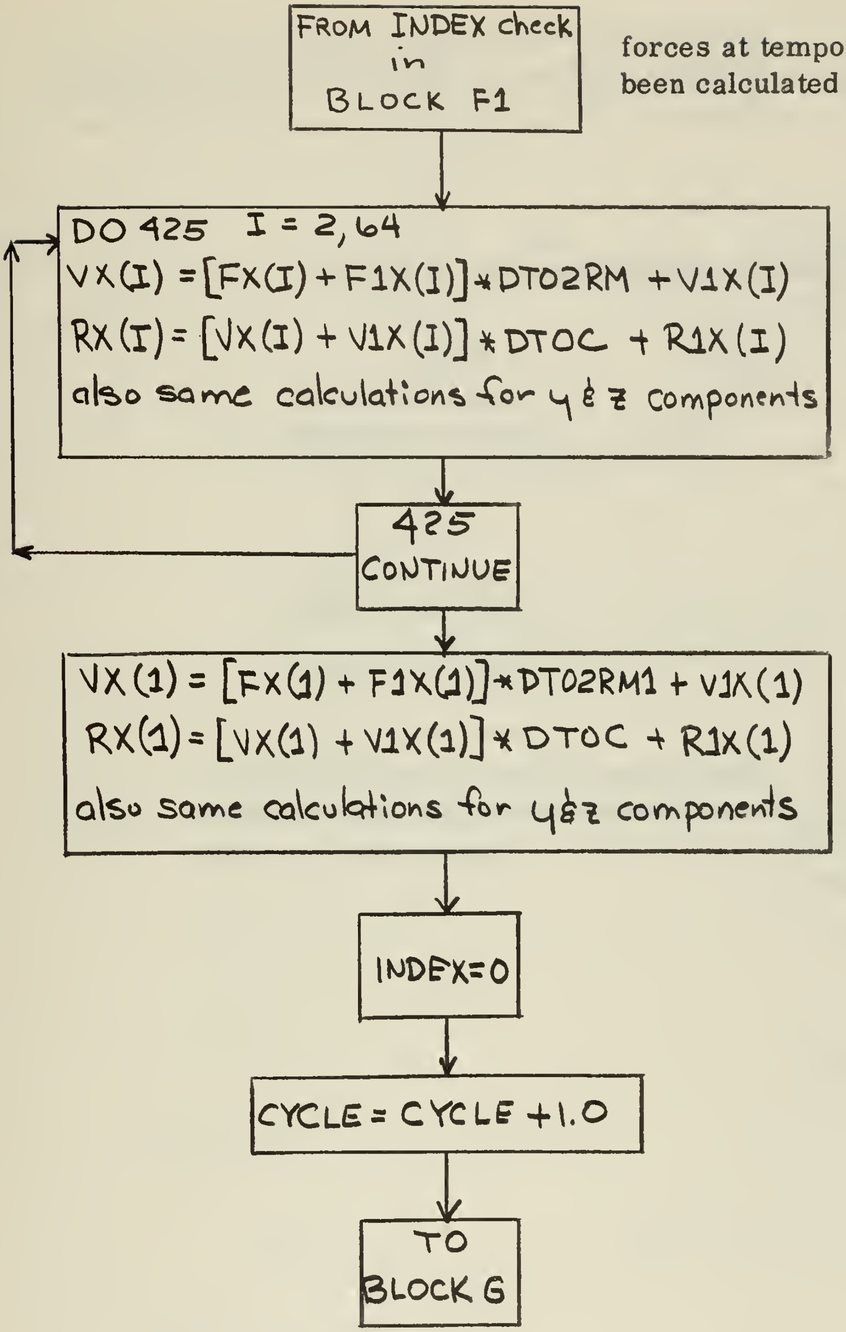
BLOCK F1 (con't)


VX(1) = FX(1) * DTORM1 + VX(1)
Also same for y & z components
RX(1) = (VX(1) + V1X(1)) * DTOC + R1X(1)
also same for y & z coordinates
INDEX = 1
GO TO 70
(IN BLOCK E)

since mass of bullet can be varied, equations of motion for the bullet must be calculated separately

recycles to calculate forces at temporary locations

BLOCK F2



```
DO 425   I = 2,64
VX(I) = [FX(I) + F1X(I)]*DTO2RM + V1X(I)
RX(I) = [VX(I) + V1X(I)]*DTOC + R1X(I)
also same calculations for y & z components
425
CONTINUE
VX(1) = [FX(1) + F1X(1)]*DTO2RM1 + V1X(1)
RX(1) = [VX(1) + V1X(1)]*DTOC + R1X(1)
also same calculations for y&z components
INDEX=0
CYCLE = CYCLE +1.0
```

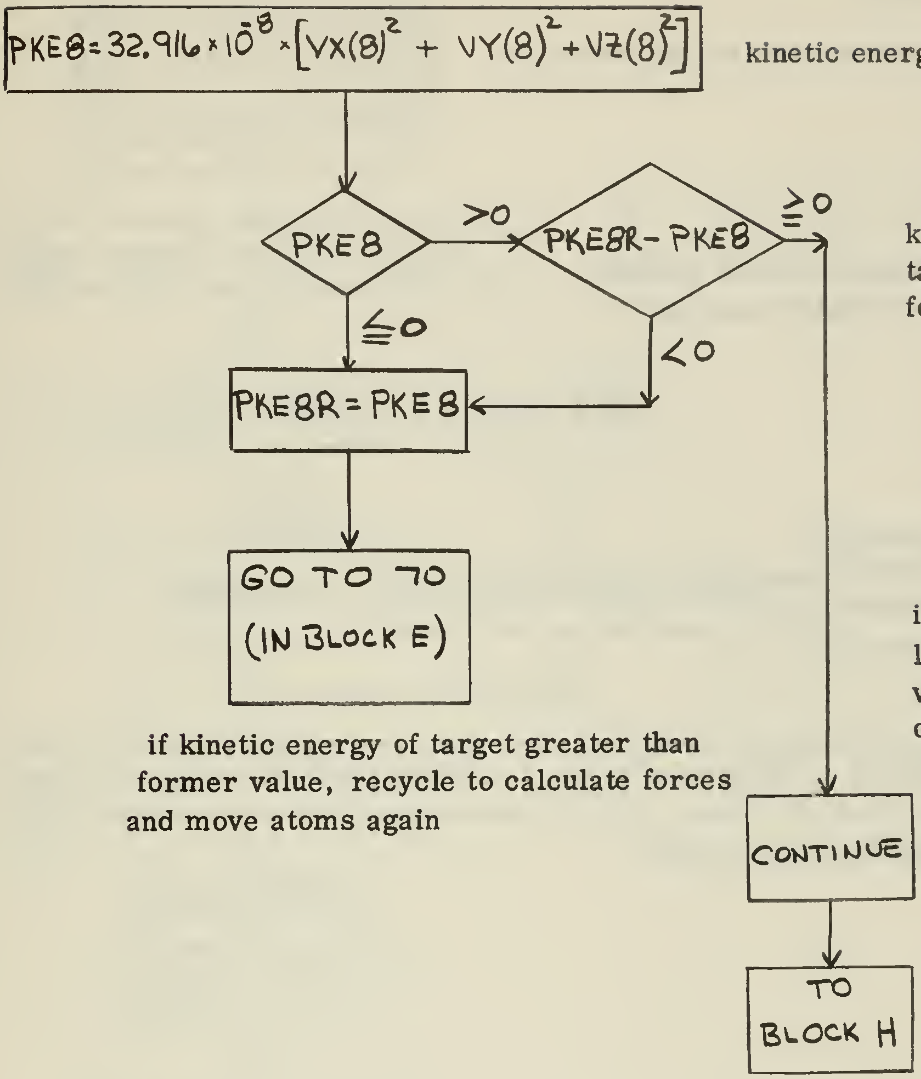
forces at temporary locations have been calculated

new velocities calculated using average forces

new positions assigned using average velocities

separate bullet calculations

BLOCK G



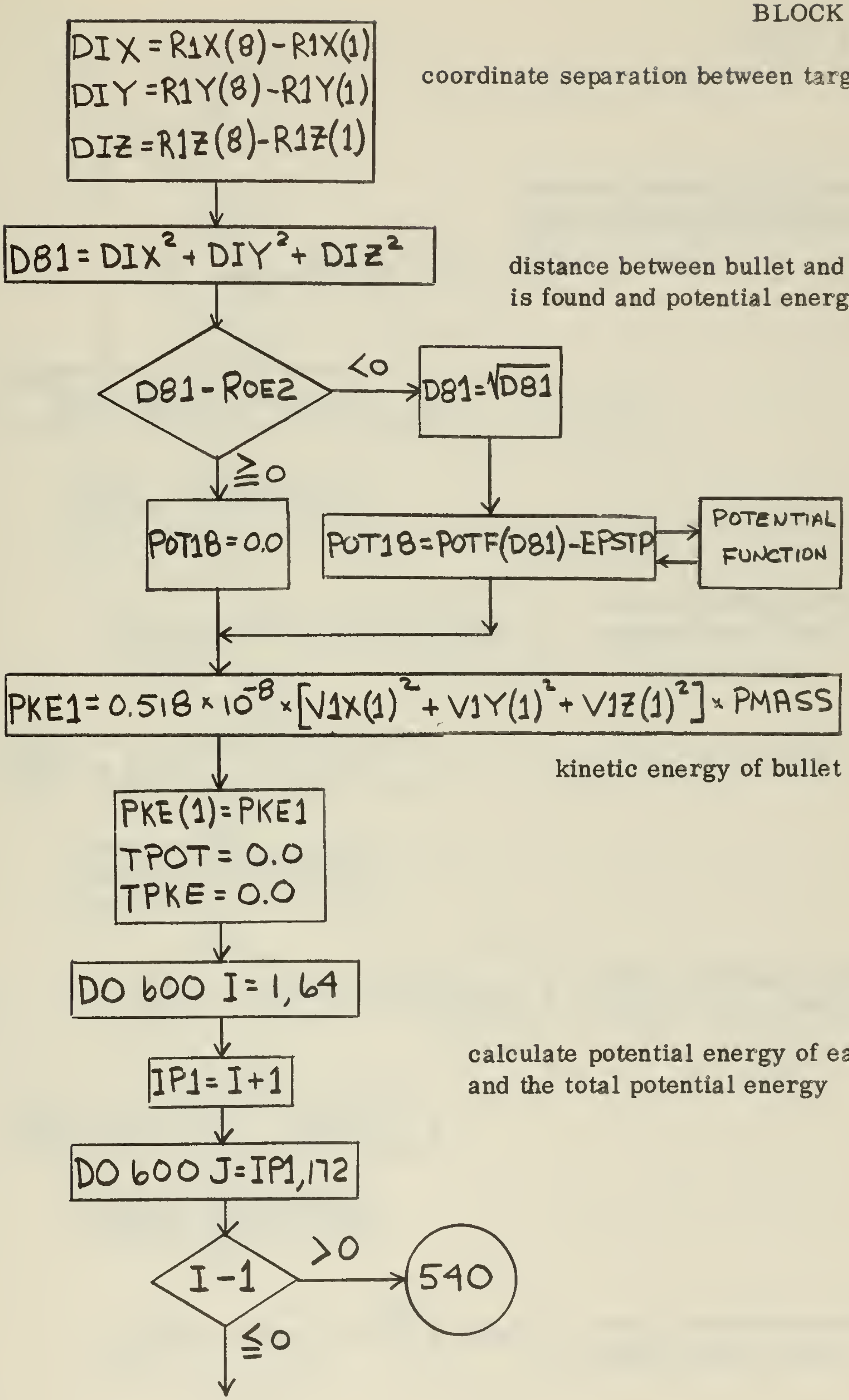
kinetic energy of target

kinetic energy of target compared to former value

if kinetic energy of target greater than former value, recycle to calculate forces and move atoms again

if kinetic energy is less than former value, movement of atoms is stopped

BLOCK H

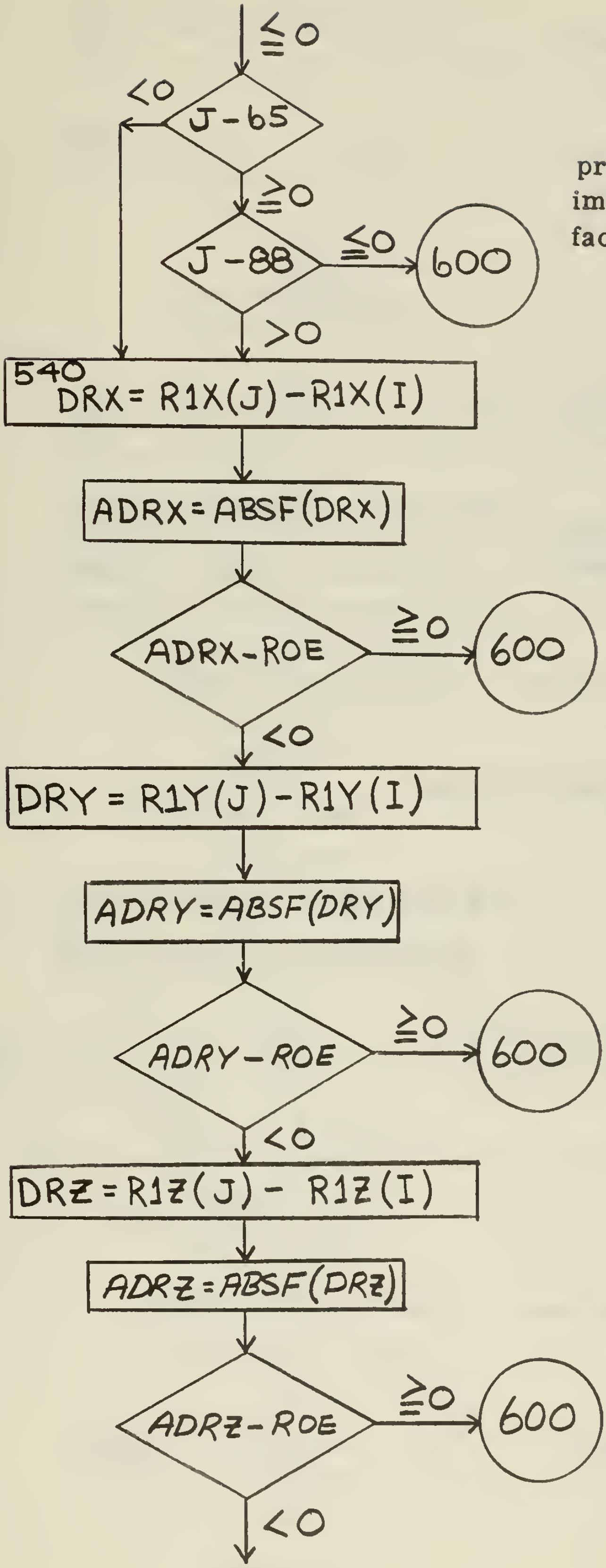


coordinate separation between target and bullet

distance between bullet and target
is found and potential energy calculated

kinetic energy of bullet

calculate potential energy of each atom
and the total potential energy



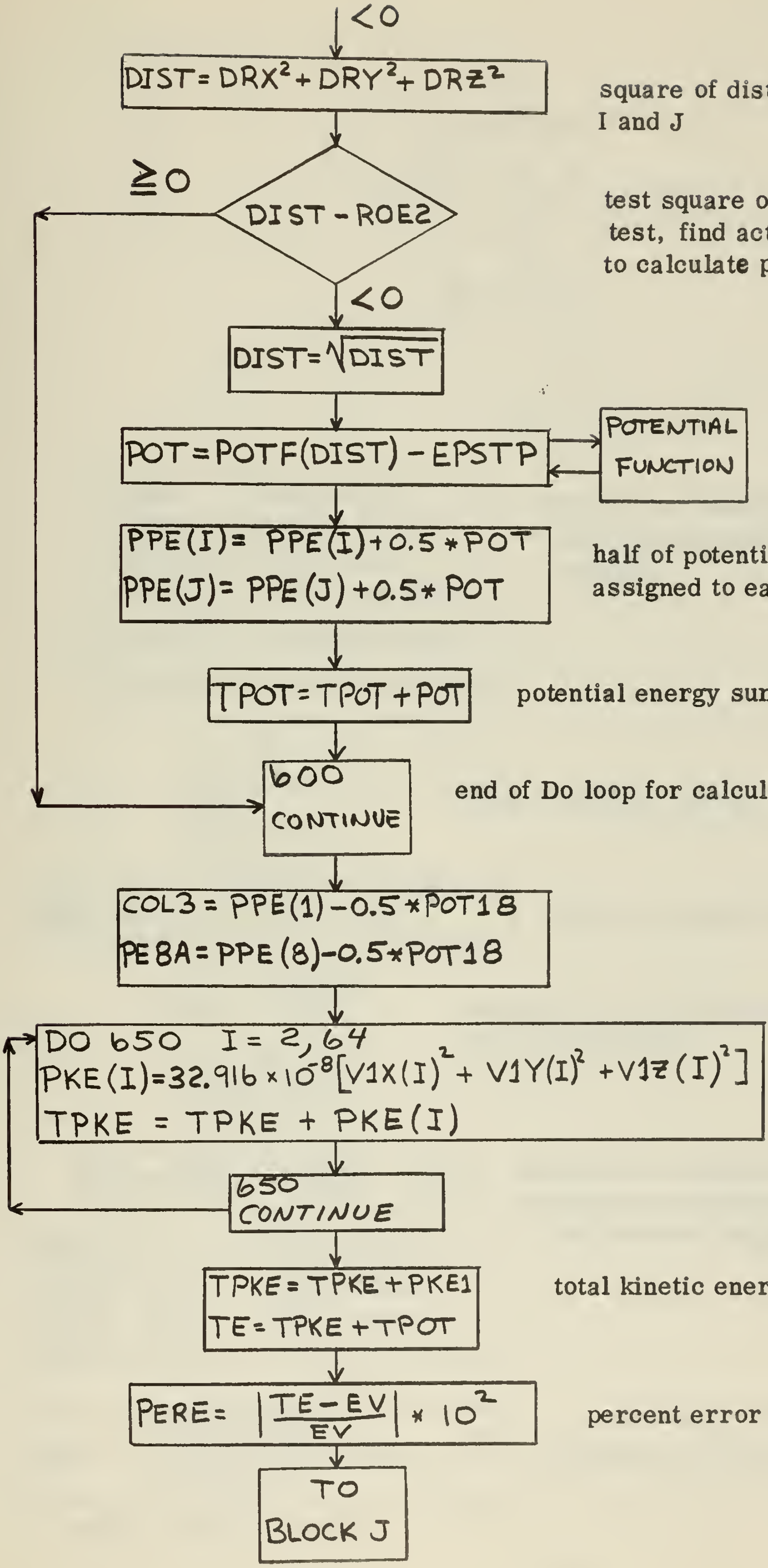
prevents interaction of bulet with immovable atoms covering bombarded face

test X coordinate separation between atom I and J

test Y coordinate separation between atom I and J

test Z coordinate separation between atom I and J

BLOCK H (con't)



<0
$DIST = DRX^2 + DRY^2 + DRZ^2$
≧0
DIST - ROE2
<0
$DIST = \sqrt{DIST}$
POT = POTF(DIST) - EPSTP
POTENTIAL FUNCTION
PPE(I) = PPE(I) + 0.5 * POT
PPE(J) = PPE(J) + 0.5 * POT
TPOT = TPOT + POT
600 CONTINUE
COL3 = PPE(1) - 0.5 * POT18
PE8A = PPE(8) - 0.5 * POT18
DO 650 I = 2, 64
$PKE(I) = 32.916 \times 10^{-8} [V1X(I)^2 + V1Y(I)^2 + V1Z(I)^2]$
TPKE = TPKE + PKE(I)
650 CONTINUE
TPKE = TPKE + PKE1
TE = TPKE + TPOT
$PERE = \left| \frac{TE - EV}{EV} \right| * 10^2$
TO BLOCK J

square of distance between atom I and J

test square of distance, if it passes test, find actual distance and use it to calculate potential between I and J

half of potential between atoms is assigned to each atom (I and J)

potential energy summation

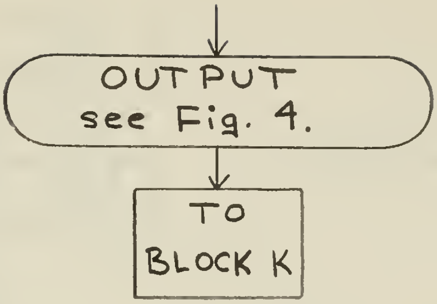
end of Do loop for calculating potential energy

kinetic energy of core atoms not including the bullet

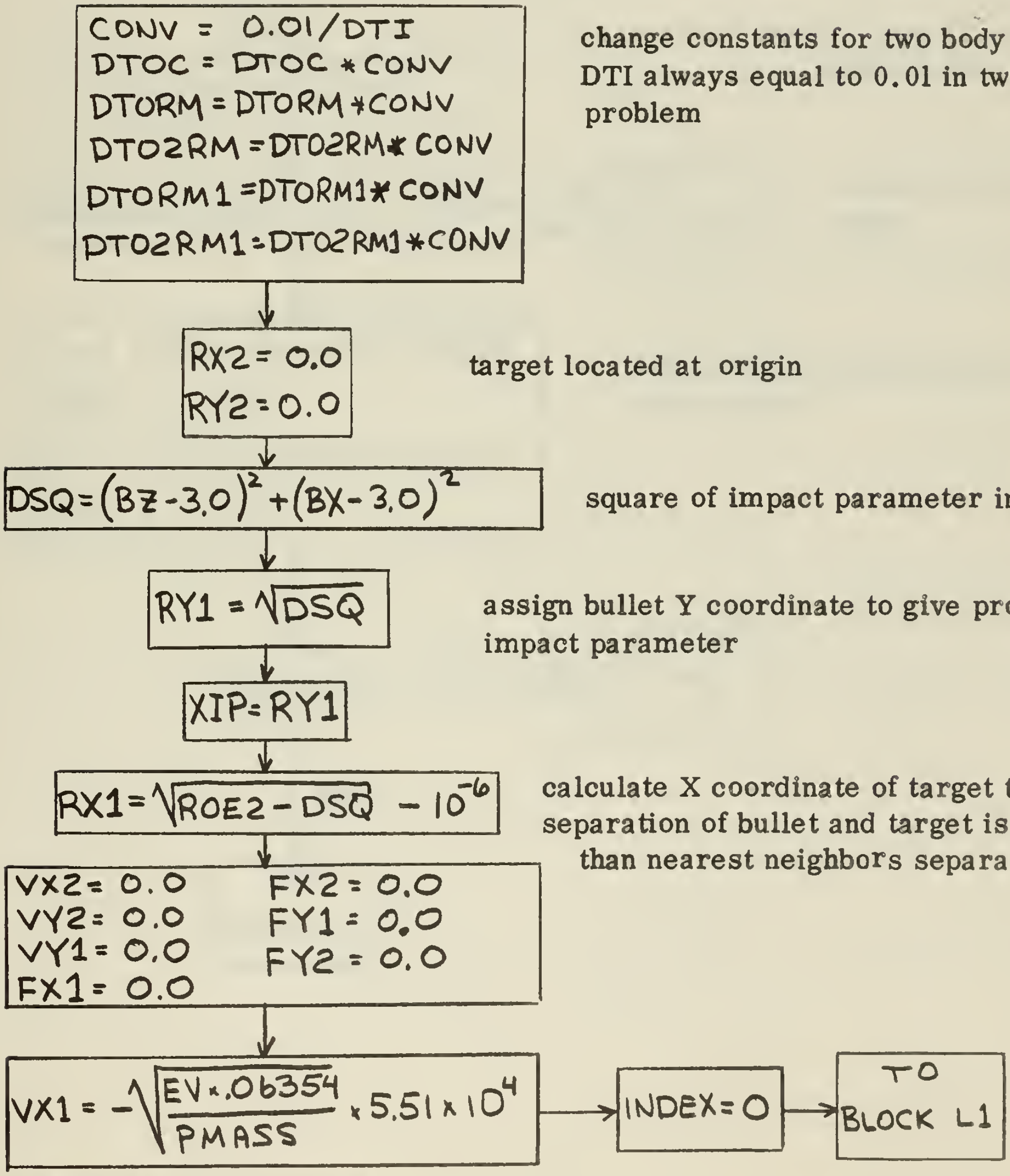
total kinetic energy and total energy

percent error in total energy

BLOCK J



BLOCK K



change constants for two body problem; DTI always equal to 0.01 in two body problem

target located at origin

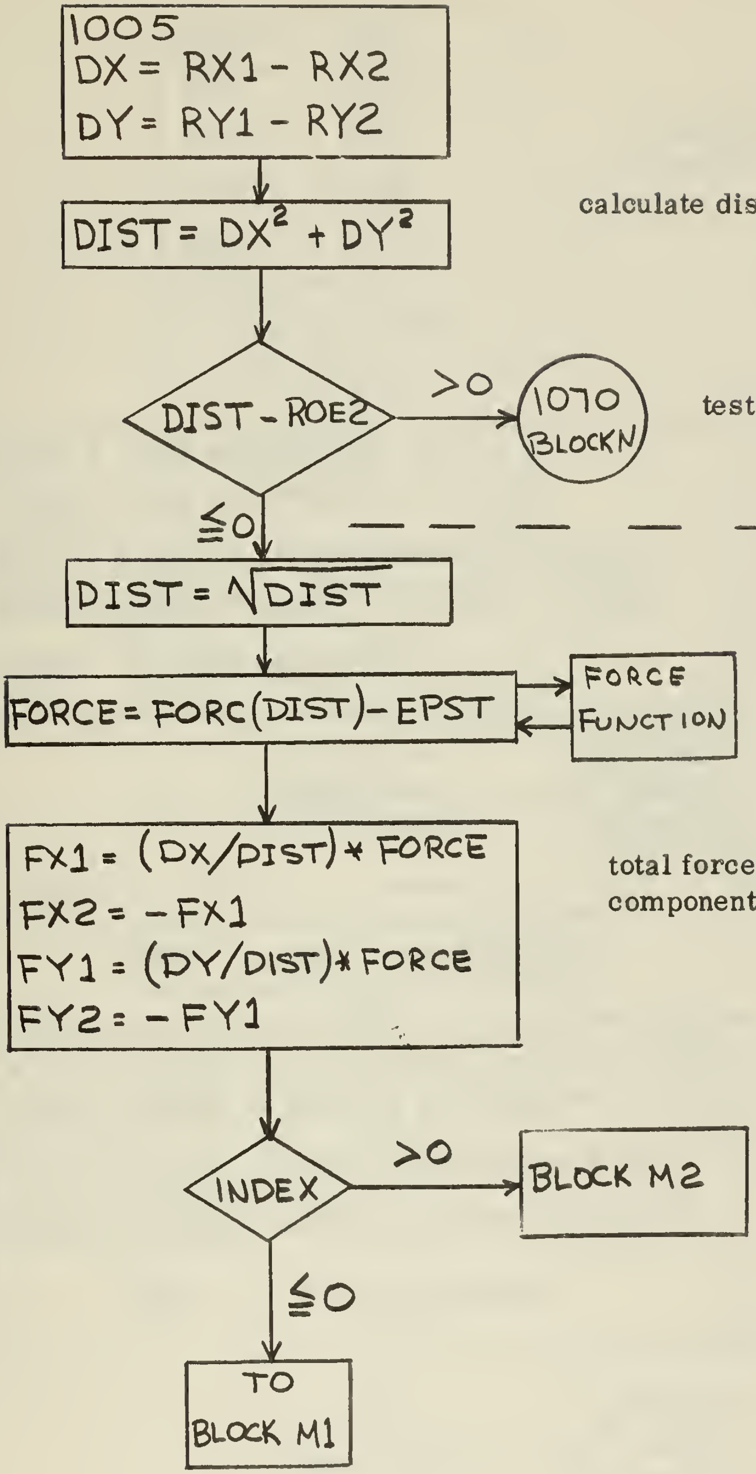
square of impact parameter in the lattice

assign bullet Y coordinate to give proper impact parameter

calculate X coordinate of target to insure separation of bullet and target is slightly less than nearest neighbors separation

assign velocity to bullet

BLOCK L1



calculate distance between atoms

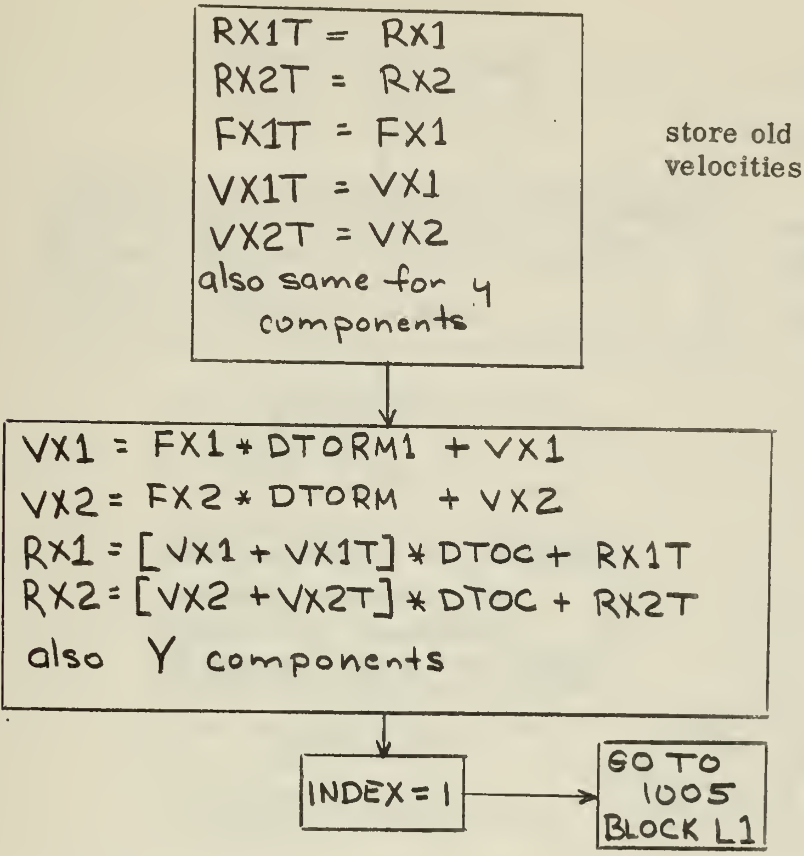
test to see if less than ROE

BLOCK L2

calculate force between atoms

total force is divided into X and Y components

BLOCK M1

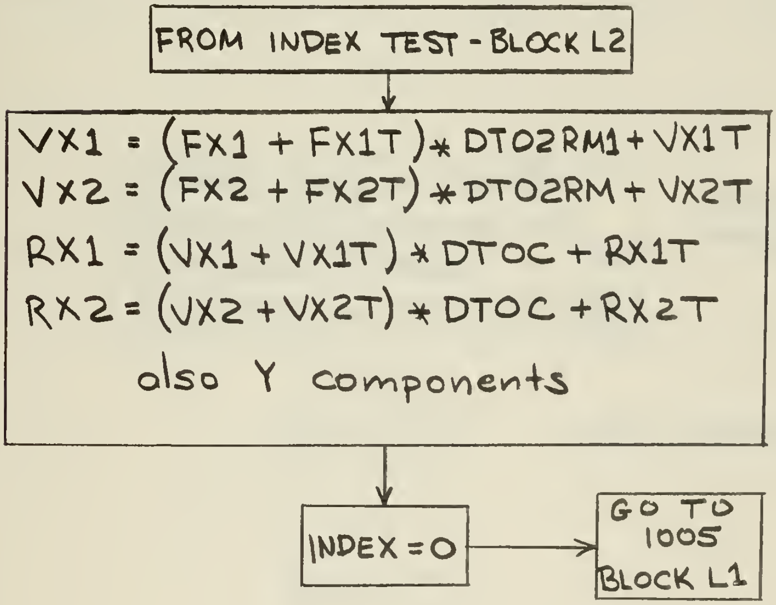


store old positions, forces, and velocities

calculate temporary velocities and positions

recycles to calculate forces at temporary positions

BLOCK M2

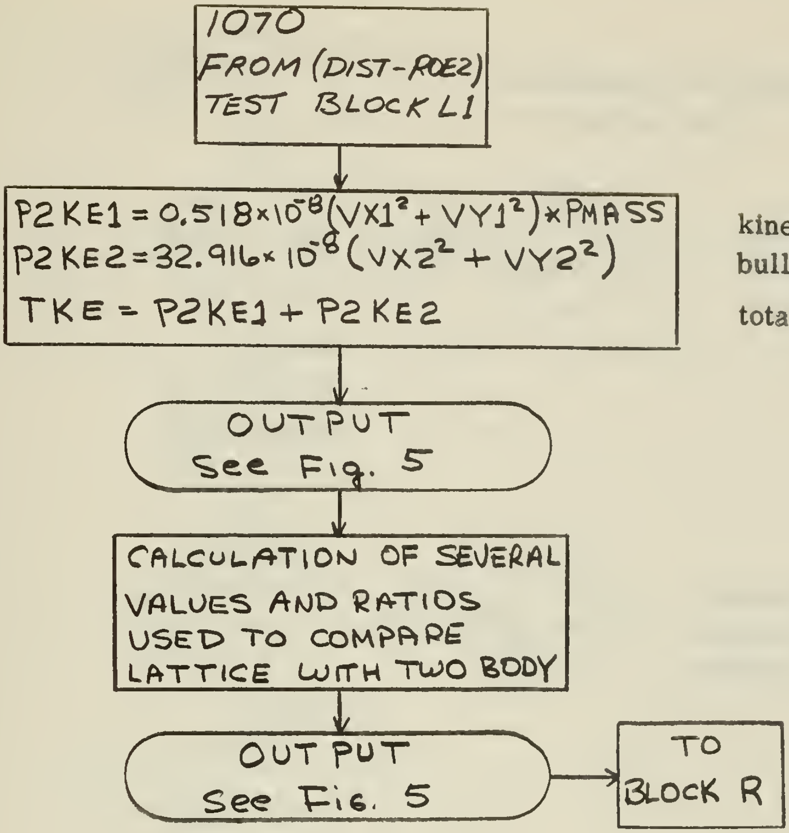

FROM INDEX TEST - BLOCK L2
VX1 = (FX1 + FX1T) * DTO2RM1 + VX1T
VX2 = (FX2 + FX2T) * DTO2RM + VX2T
RX1 = (VX1 + VX1T) * DTOC + RX1T
RX2 = (VX2 + VX2T) * DTOC + RX2T
also Y components
INDEX = 0
GO TO 1005 BLOCK L1

calculate final velocities and positions

average forces and velocities are used

recycles to distance test

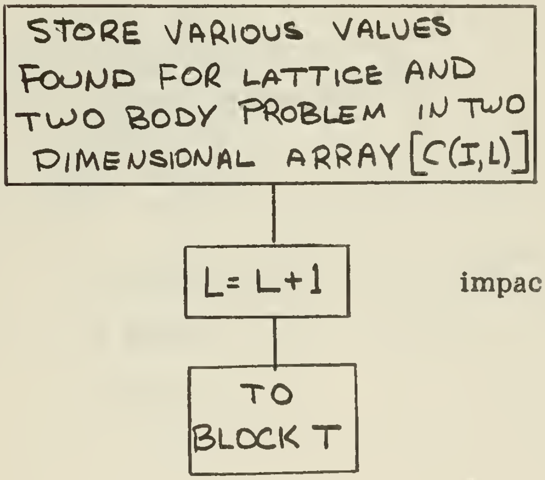
BLOCK N


1070
FROM (DIST-ROE2)
TEST BLOCK L1
P2KE1 = 0.518×10⁻⁸(VX1² + VY1²)×PMASS
P2KE2 = 32.916×10⁻⁸(VX2² + VY2²)
TKE = P2KE1 + P2KE2
OUTPUT
See Fig. 5
CALCULATION OF SEVERAL VALUES AND RATIOS USED TO COMPARE LATTICE WITH TWO BODY
OUTPUT
See Fig. 5
TO
BLOCK R

kinetic energy of target and bullet

total energy of system

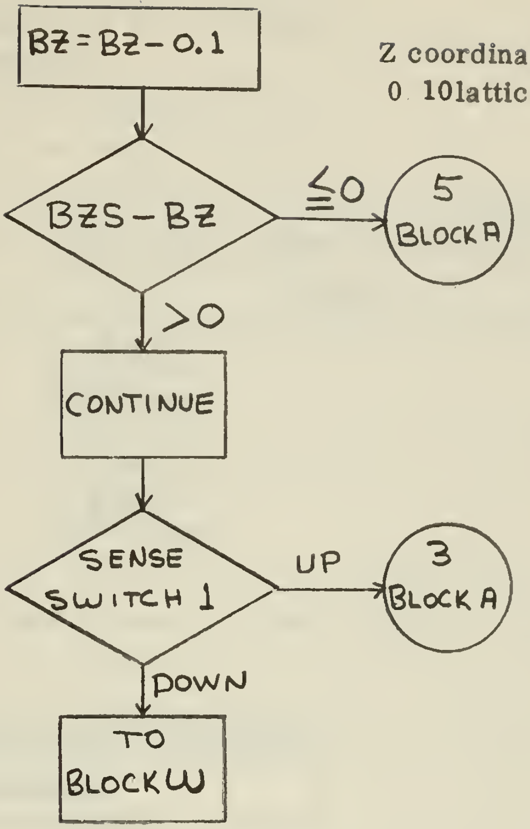
BLOCK R


STORE VARIOUS VALUES FOUND FOR LATTICE AND TWO BODY PROBLEM IN TWO DIMENSIONAL ARRAY [C(I,L)]
L = L+1
TO
BLOCK T

index I is value stored
index L is impact point number

impact point number increased by one

BLOCK T

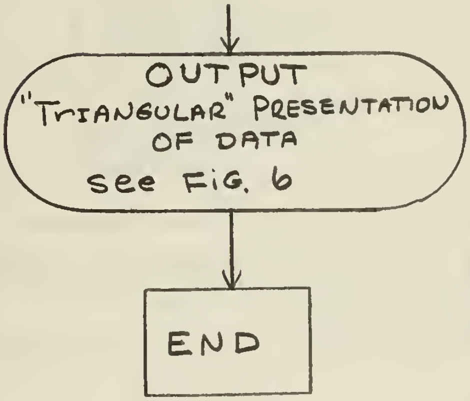


Z coordinate of impact point lowered by 0.10 lattice units

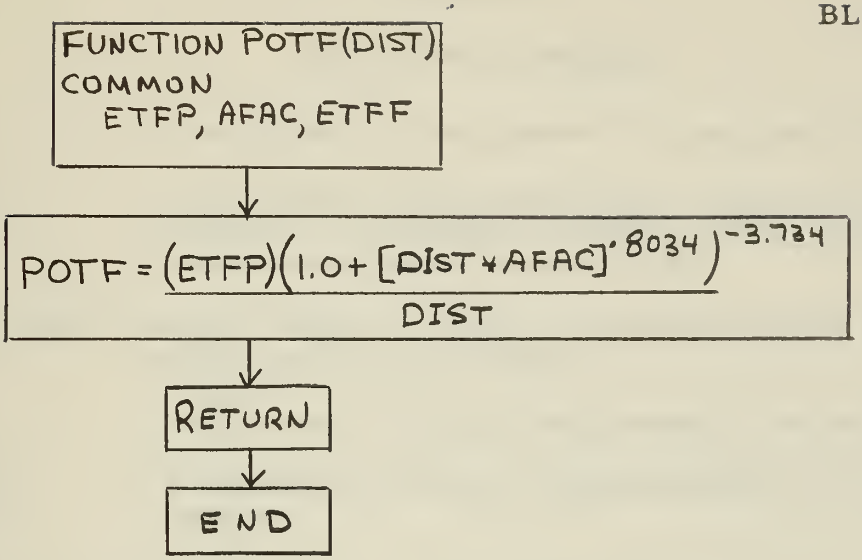
Z coordinate of impact point tested to see if it is the end of a column

if sense switch one is up, new data card is read to start another column in "triangle"

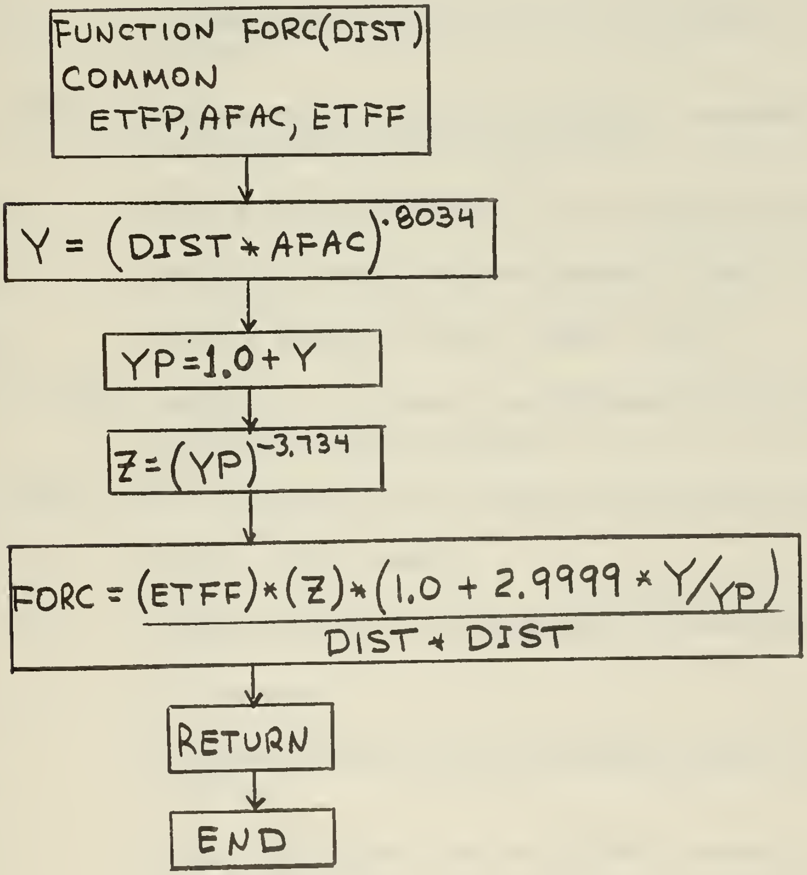
BLOCK W



BLOCK Y



BLOCK Z



APPENDIX IV

DEFINITION OF VARIABLES

RX(I)	X coordinate of atom number I at any time (lattice units)
R1X(I)	x coordinate of atom number I at former position (same as position 1 in procedure section), stored while average forces are computed (lattice units)
RY(I), RZ(I), R1Y(I), R1Z(I)	y and z coordinates defined in the same manner as RX(I) and R1X(I)
FX(I)	x component of force on atom number I at any time (newtons)
F1X(I)	x component of force at former position of atom number I (newtons)
FY(I), FZ(I), F1Y(I), F1Z(I)	y and z components of force defined in the same manner as FX(I) and F1X(I)
VX(I)	x component of velocity at any time of atom number I (m/sec)
V1X(I)	x component of velocity of atom number I at former position (m/sec)
VY(I), VZ(I), V1Y(I), V1Z(I)	y and z velocity components defined in the same manner as VX(I) and V1X(I)
C(I,L)	matrix for storing data I from impact point L
PPE(I)	potential energy of atom number I (ev)
PKE(I)	kinetic energy of atom number I (ev)
RXR(I), RYR(I), RZR(I)	x, y, and z coordinates of all atoms in initial positions (lattice units)
ETFP, AFAC, ETFF	constants used in Thomas-Fermi-Firsov potential
L	impact point number
ROE	nearest neighbors separation (lattice units)
ROE2	ROE squared
EPST	value subtracted from calculated force to erode the force (newtons)
EPSTP	value subtracted from calculated potential to erode the potential (ev)

FORC	function subroutine that calculates force; argument is the separation of atoms (newtons)
POTF	function subroutine that calculates potential; argument is the separation of atoms (ev)
EV	original kinetic energy of bullet (ev)
BX	original x coordinate of bullet (lattice units)
DTI	time step multiplier
PMASS	mass of the bullet (amu)
BZ	original z coordinate of bullet (lattice units)
BZS	z coordinate of bullet at end of column in impact triangle, used as stopping point (lattice units)
PKE8R	kinetic energy of target at the end of previous time step (ev)
CYCLE	number of time steps
INDEX	switching device
DT	length of basic time step (seconds)
RM	mass of copper atom (kg)
RM1	mass of bullet atom (kg)
DTOC	a constant used in movement equations; when multiplied by the sum of two velocities, it computes the average, multiplies it by DT and gives the result in lattice units (sec x lattice units/m)
DTORM	a constant used in velocity equations; it combines the quotient DT/RM into one constant to avoid repeated divisions (sec/kg)
DTO2RM	same as DTORM except it averages the force
DTORM1	same as DTORM but used in bullet calculations only, since the bullet mass may be different from that of the lattice atoms
DTO2RM1	same as DTO2RM but used in bullet calculations only since bullet mass may be different from that of the lattice atoms
M,N	atom numbers
JT	y coordinate of an x-z plane

KT	z coordinate of an x-y plane
IT	x coordinate of a y-z plane
NTC	sum of x,y, and z coordinates of a point in the lattice
DRX,DRY,DRZ	difference between x,y, and z coordinates respectively of any two atoms (lattice units)
ADRX, ADRY, ADRZ	absolute value of DRX, DRY, and DRZ
DIST	distance between two atoms or the square of the distance (lattice units)
FORCE	eroded force between two atoms (newtons)
FOD	FORCE divided by the distance between two atoms (newtons/lattice unit)
FA,FB,FC	x,y, and z components respectively of the force between two atoms (newtons)
PKE8	kinetic energy of target atom in the lattice (ev)
DIX,DIY,DIZ	x,y, and z coordinate separation between target and bullet (lattice units)
D81	distance between target and bullet in lattice or the square of the distance (lattice units)
POT18	potential between target and bullet (ev)
PKE1	kinetic energy of bullet at end of time step (ev)
TPOT	total potential energy of lattice (ev)
TPKE	total kinetic energy of lattice (ev)
POT	potential between any two atoms (ev)
COL3	potential of the bullet with respect to the lattice minus the target (ev)
PE8A	potential energy of the target with respect to the lattice minus the bullet (ev)
TE	total energy of the lattice (ev)
PERE	percent error in total energy (percent)
CONV	time step multiplier conversion factor for two body problem; makes two body time step multiplier equal to 0.01 regardless of the value used for the lattice problem

DSQ	square of the impact parameter in the two body problem (lattice units squared)
XIP	impact parameter in the two body problem (lattice units)
RX2, RY2	x and y coordinates of target at any time in two body problem (lattice units)
RX2T, RY2T	x and y coordinates of target at former position, stored while average force is computed (lattice units)
RX1, RY1, RX1T, RY1T	x and y coordinates of the bullet in the two body problem defined in the same manner as RX2, RY2, RX2T, and RY2T
VX2, VY2	x and y components of target velocity in two body problem (m/sec)
VX2T, VY2T	x and y components of target velocity in two body problem at former position (m/sec)
VX1, VY1, VX1T, VY1T	x and y components of velocity of the bullet in the two body problem defined in the same manner as VX2, VY2, VX2T, and VY2T
FX1, FY1	x and y components of force on the bullet in the two body problem (newtons)
FX1T, FY1T	x and y components of force on the bullet in the two body problem at its former position (newtons)
FX2, FY2, FX2T, FY2T	x and y components of force on the target in the two body problem defined in the same manner as FX1, FY1, FX1T, and FY1T
DX	x coordinate separation between atoms in the two body problem (lattice units)
DY	y coordinate separation between atoms in the two body problem (lattice units)
P2KE1	kinetic energy of the bullet in the two body problem after interaction is complete (ev)
P2KE2	kinetic energy of the target in the two body problem after interaction is complete (ev)
TKE	total kinetic energy in the two body problem (ev)
T2RA	recoil angle in the two body problem (degrees)
B2SA	scattering angle in the two body problem (degrees)

SRE8	resultant velocity of target in lattice (m/sec)
SRE1	resultant velocity of bullet in lattice (m/sec)
ATLRA	quotient of two velocities; used to find TLRA
TLRA	recoil angle in the lattice (degrees)
ABLSA	quotient of two velocities; used to find BLSA
BLSA	scattering angle in the lattice (degrees)
RBMT	bullet to target mass ratio
EABL	energy absorbed by the lattice; does not include potential or kinetic energy of target and bullet (ev)
ET2,ETL,RET,RKEP,RSA2L,RRA2L,RBFI	ratios used to compare lattice interaction with two body problem; the ratios are in terms of variables already defined.

APPENDIX V

PROGRAM LISTING

BLOCK A

```
      PROGRAM TFF
      DIMENSION RX(200), RY(20C), RZ(200)
      DIMENSICN  FX(200),FY(2CC),FZ(200)
      DIMENSION   VX(200) , VY(2CC) , VZ(2C0)
     ODIMENSION  R1X(2C0), R1Y(2CC), R1Z(200), F1X(20C), F1Y(2CC),
     1  F1Z(200) , V1X(200), V1Y(200), V1Z(2CC)
      DIMENSION C(22,36 ),PPE(200),PKE(200),RXR(200),RYR(200),RZR(200)
      COMMCN ETFP,AFAC,ETFF
      AFAC=3.5906
      ETFF=5.9360E-6
      ETFP=6.6980E+3
      L=1
      ROE = SQRTF (2.0)
      ROE2 = 2.C
      EPST = FORC ( ROE )
      EPSTP = POTF(ROE)
 10   FORMAT(34X54H THOMAS-FERMI-FIRSOV POTENTIAL, ERCDED, CCPPER-COPPER
     1         )
    3 READ INPUT TAPE 2,4, EV,BX,DTI, PMASS
  4   FORMAT(4E10.3)
      BZ = BX + 1.0
      BZS = 6.0-BX
 5    RX(1) = BX
      RZ(1) = BZ
      PKEBR = -100.0
      CYCLE = 0.0
      INDEX = 0
      RY(1) = -SQRTF(2.0)
 12  OFORMAT(/,29H BULLET INCOMING LOCATION  X= F6.3, 5H   Z= F6.3,
     110H   ENERGY= F8.1, 24H   TIME STEP MULTIPLIER=  F5.3, /  )
 15   FORMAT(1H1)
```

BLOCK B

```
      VX(1) = 0.C
      VY(1)= SQRTF( EV * 63.54/(1.CE3 * PMASS) ) * 5.511811 E04
      VZ(1) = 0.0
      DT =  DTI/ VY(1) * 1.807E-10
      RM= 105.463911 E-27
      DTOC  = DT/3.614 E-10
      DTORM =  DT / RM
      DTO2RM = DTORM/2.0
      RM1 = PMASS *1.6598 E-27
      DTORM1 = DT/RM1
      DTO2RM1  = DTORM1/ 2.0
      DO 250 I = 2, 64
      VX(I) = 0.0
      VY(I) = 0.0
 250  CONTINUE
```

BLOCK C

```
      M = 2
      N = 65
      JT = -1
      DO 60 J = 1,7
      KT = 0
      DO 59 K = 1,7
      IT = 0
      DO 58 I = 1,7
      NTC=IT+JT+KT
      IF(NTC-NTC/2*2) 57,20,57
   20 IF(KT - 1) 30, 21, 21
   21 IF(KT -5) 22, 22, 30
   22 IF(IT - 1) 30, 23, 23
   23 IF(IT - 5) 24, 24, 30
   24 IF(JT-0) 30, 25 , 25
   25 IF(JT-4) 40, 40, 30
   30 RX(N) = IT
      RY(N) = JT
      RZ(N) = KT
      N = N + 1
      GO TO 57
   40 RX(M)=IT
      RY(M) = JT
      RZ(M) = KT
      M = M+ 1
   57 IT=IT+1
   58 CONTINUE
      KT = KT + 1
   59 CONTINUE
      JT = JT + 1
   60 CONTINUE
```

BLOCK D

```
      DO 65 I = 65, 172
      PPE(I)=0.0
      R1X(I) = RX(I)
      R1Y(I) = RY(I)
      R1Z(I) = RZ(I)
 65   CONTINUE
      DO 66  I= 1,64
      PPE(I)=0.0
      PKE(I)=0.0
      RXR(I) =RX(I)
      RYR(I)=RY(I)
   66 RZR(I) = RZ(I)
```

BLOCK E

```
  70 DO 75  I = 1, 64
     FX(I)= 0.0
     FY(I) = 0.0
     FZ(I) = 0.0
  75 CONTINUE
     DO 200 I = 1,64
     IP1 = I + 1
     DO 200 J = IP1 , 172
     IF (I-1) 130,130, 120
 130 IF(J-65) 120,135, 135
 135 IF(J-88) 200, 200, 120
 120 DRX = RX(J) - RX(I)
     ADRX = ABSF (DRX)
     IF(ADRX - ROE) 140,200,200
140  DRY = RY(J) - RY(I)
     ADRY = ABSF(DRY)
     IF(ADRY - ROE) 145,200,200
145  DRZ = RZ(J) - RZ(I)
     ADRZ = ABSF(DRZ)
     IF(ADRZ - ROE) 150,200,200
150  DIST = (DRX * DRX   + DRY*DRY +   DRZ * DRZ )
     IF ( DIST - ROE2)   155, 200, 200
 155 DIST = SQRTF( DIST)
     FORCE = FORC( DIST) - EPST
     FOD = FORCE / DIST
     FA = DRX * FOD
     FB = DRY * FOD
     FC = DRZ * FOD
     IF( J-65) 160,165,165
 160 FX(J) = FX(J) + FA
     FY(J) = FY(J) + FB
     FZ(J) = FZ(J) + FC
 165 FX(I) = FX(I) - FA
     FY(I) = FY(I) - FB
     FZ(I) = FZ(I) - FC
 200 CONTINUE
     DO 235 I = 1,64
     IF( ABSF(FX(I)) -1.0E-14) 210, 210, 215
 210 FX(I) = 0.0
 215 IF( ABSF(FY(I)) -1.0E-14) 220, 220, 225
 220 FY(I) = 0.0
 225  IF( ABSF(FZ(I)) -1.0E-14) 230, 230, 235
 230 FZ(I) = 0.0
 235 CONTINUE
     IF (INDEX)  240, 240, 420
```

```
                                    BLOCK F1

240 DO 300 I = 2, 64
    R1X(I) = RX(I)
    R1Y(I) = RY(I)
    R1Z(I) = RZ (I)
    F1X(I) =  FX(I)
    F1Y(I) =  FY(I)
    F1Z(I) =  FZ(I)
    V1X(I) = VX(I)
    V1Y(I) = VY(I)
    V1Z(I) = VZ(I)
    VX(I) = FX(I) * DTORM  +  VX(I)
    VY(I) = FY(I) * DTORM  +  VY(I)
    VZ(I) = FZ(I) *DTORM  +  VZ(I)
    RX(I) = ( VX(I) + V1X(I)) * DTOC   +  R1X(I)
    RY(I) = ( VY(I) + V1Y(I)) * DTOC   +  R1Y(I)
    RZ(I) = ( VZ(I) + V1Z(I)) * DTOC   +  R1Z(I)
300 CONTINUE
    R1X(1) = RX(1)
    R1Y(1) = RY(1)
    R1Z(1) = RZ(1)
    F1X(1) = FX(1)
    F1Y(1) = FY(1)
    F1Z(1) = FZ(1)
    V1X(1) = VX(1)
    V1Y(1) = VY(1)
    V1Z(1) = VZ(1)
    VX(1) = FX(1) * DTORM1  +  VX(1)
    VY(1) = FY(1) * DTORM1  + VY(1)
    VZ(1) = FZ(1) * DTORM1  + VZ(1)
    RX(1) = ( VX(1) + V1X(1) ) * DTOC   +  R1X(1)
    RY(1) = ( VY(1) + V1Y(1) ) *DTOC   +  R1Y(1)
    RZ(1) = ( VZ(1) + V1Z(1)) * DTOC   +  R1Z(1)
    INDEX = 1
    GO TO 70

                                    BLOCK F2

420  DO 425  I = 2,64
    VX(I) = ( FX(I) + F1X(I)) *DTO2RM   +  V1X(I)
    VY(I) = ( FY(I) + F1Y(I)) *DTO2RM  +  V1Y(I)
    VZ(I) = ( FZ(I) + F1Z(I)) *DTO2RM   +  V1Z(I)
    RX(I) = ( VX(I) + V1X(I)) * DTOC   +  R1X(I)
    RY(I) = ( VY(I) + V1Y(I)) * DTOC   +  R1Y(I)
    RZ(I) = ( VZ(I) + V1Z(I)) * DTOC   +  R1Z(I)
425 CONTINUE
    VX(1) = (FX(1) + F1X(1)) *DTO2RM1   +   V1X(1)
    VY(1) = (FY(1) + F1Y(1)) * DTO2RM1  + V1Y(1)
    VZ(1) = ( FZ(1) + F1Z(1)) * DTO2RM1 +   V1Z(1)
    RX(1) = ( VX(1) + V1X(1) ) * DTOC   +  R1X(1)
    RY(1) = ( VY(1) + V1Y(1) ) *DTOC   +  R1Y(1)
    RZ(1) = ( VZ(1) + V1Z(1)) * DTOC   +  R1Z(1)
    INDEX = 0
    CYCLE = CYCLE  + 1.0

                                    BLOCK G

    PKE8 =32.9163268E-08*(VX(8)*VX(8) + VY(8)*VY(8) + VZ(8)*VZ(8) )
    IF(PKE8) 460, 460,455
455 IF(PKE8R-PKE8)  460,465,465
460 PKE8R = PKE8
    GO TO 70
465 CONTINUE
```

BLOCK H

```
      DIX = R1X(8) - R1X(1)
      DIY = R1Y(8) - R1Y(1)
      DIZ = R1Z(8) - R1Z(1)
      D81 = (DIX*DIX + DIY*DIY + DIZ*DIZ)
      IF(D81 - ROE2) 428,435,435
 428  D81 = SQRTF(D81)
  430 POT18 = POTF(D81) - EPSTP
      GO TO 440
  435 POT18 = 0.0
  440 PKE1 = 0.51804102E-08*(V1X(1)*V1X(1) + V1Y(1)*V1Y( 1) + V1Z(1) *
     1V1Z(1))*PMASS
      PKE(1) = PKE1
      TPOT = 0.0
      TPKE = 0.0
      DO 600  I = 1,64
      IP1 = I + 1
      DO 600  J =IP1,172
      IF( I -1)  525 , 525 , 540
  525 IF( J-65) 540 ,530, 530
  530 IF(J - 88) 600 , 600,540
  540 DRX = R1X(J) - R1X(I)
      ADRX = ABSF(DRX)
      IF(ADRX - ROE) 545,600,600
 545  DRY = R1Y(J) - R1Y(I)
      ADRY = ABSF(DRY)
      IF(ADRY - ROE) 550,600,600
 550  DRZ = R1Z(J) - R1Z(I)
      ADRZ = ABSF(DRZ)
      IF(ADRZ - ROE) 555,600,600
 555  DIST = (DRX*DRX + DRY*DRY + DRZ*DRZ)
      IF(DIST - ROE2) 556,600,600
 556  DIST = SQRTF(DIST)
  560 POT = POTF(DIST) - EPSTP
      PPE(I)=PPE(I) + 0.5* POT
      PPE(J) = PPE(J) + 0.5 * POT
      TPOT = TPOT + POT
  600 CONTINUE
      COL3 = PPE(1) - 0.5 * POT18
      PE8A=PPE(8) -0.5 * POT18
      DO 650  I=2,64
      PKE(I)=32.9165268E-08*(V1X(I)*V1X(I)+V1Y(I)*V1Y(I)+V1Z(I)*V1Z(I))
      TPKE = TPKE + PKE(I)
  650 CONTINUE
      TPKE = TPKE + PKE1
      TE = TPKE  + TPOT
      PERE  = ABSF((TE-EV)/EV) *1.0E2
```

BLOCK J

```
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3, 12, BX, BZ, EV, DTI
      WRITE OUTPUT TAPE 3, 850
  850 FORMAT( /,  19H LATTICE LOCATIONS ,/)
      WRITE OUTPUT TAPE 3,860
  860 FORMAT(90H    ATOM          DX          DY          DZ          VX          VY
     1         VZ          KE          PE          /)
      SHIFT = 1.0E-05
      DO 900 I= 1,64
      ENI2(0).
      DX=R1X(I)-RXR(I)
      +SSK(DX),SLJ(L+2),+SCM(77777B),+FSB(SHIFT),AJP3(865),INI2(1).
  865 DY= R1Y(I) - RYR(I)
      +SSK(DY),SLJ(L+2),+SCM(77777B),+FSB(SHIFT),AJP3(875),INI2(1).
  875 DZ= R1Z(I)- RZR(I)
      +SSK(DZ),SLJ(L+2),+SCM(77777B),+FSB(SHIFT),AJP3(885),INI2(1).
  885 ENA2(0),AJP(900).
  890 WRITE OUTPUT TAPE 3,895,I,DX,DY,DZ,V1X(I),V1Y(I),V1Z(I),PKE(I),
     1PPE(I)
  900 CONTINUE
 895  FORMAT(I10,3F10.5,3E10.2,2F10.2)
```

```
                                    BLOCK K

      CONV = 0.01/DTI
      DTOC = DTOC * CONV
      DTORM =  DTORM * CONV
      DTO2RM = DTO2RM * CONV
      DTORM1=DTORM1 *CONV
      DTO2RM1 = DTO2RM1 * CONV
      RX2 =0.0
      RY2 = 0.0
      DSQ=(BZ-3.0)*(BZ-3.0)+(BX-3.0)*(BX-3.0)
      RY1= SQRTF(DSQ)
      XIP=RY1
      RX1= SQRTF(ROE2-DSQ) - 1.0E-06
      VX2 = 0.0
      VY2 = 0.0
      VY1 = 0.0
      FX1 = 0.0
      FX2= 0.0
      FY1= 0.0
      FY2= 0.0
      VX1 = -SQRTF(EV * 0.06354 / PMASS) * 5.511811E04
      INDEX = 0

                                    BLOCK L1

 1005 DX = RX1- RX2
      DY = RY1- RY2
      DIST = DX*DX + DY*DY
      IF(DIST-ROE2) 1010, 1010, 1070

                                    BLOCK L2

 1010 DIST = SQRTF(DIST)
      FORCE= FORC(DIST) - EPST
      FX1 = DX/ DIST * FORCE
      FX2 = -FX1
      FY1=  DY/DIST * FORCE
      FY2 = - FY1
      IF(INDEX) 1015,1015,1030

                                    BLOCK M1

 1015 RX1T = RX1
      RY1T = RY1
      RX2T = RX2
      RY2T = RY2
      FX1T = FX1
      FY1T = FY1
      FX2T = FX2
      FY2T = FY2
      VX1T = VX1
      VY1T = VY1
      VX2T = VX2
      VY2T= VY2
      VX1 = FX1 * DTORM1 +  VX1
      VY1 = FY1 * DTORM1  + VY1
      VX2 = FX2 * DTORM  + VX2
      VY2 = FY2 * DTORM  +  VY2
      RX1 = (VX1 + VX1T)* DTOC  +  RX1T
      RY1 = (VY1 + VY1T) * DTOC  +  RY1T
      RX2 = (VX2 + VX2T) * DTOC   + RX2T
      RY2 = (VY2 + VY2T) *DTOC   + RY2T
      INDEX = 1
      GO TO 1005
```

```
                                  BLOCK M2

1030 VX1= (FX1  + FX1T)* DTO2RM1 +  VX1T
     VY1 = (FY1 + FY1T)* DTO2RM1  + VY1T
     VX2= (FX2  + FX2T)* DTO2RM    + VX2T
     VY2= (FY2  + FY2T)*DTO2RM    +  VY2T
     RX1 = (VX1 + VX1T)* DTOC  +  RX1T
     RY1 = (VY1 + VY1T) * DTOC  +  RY1T
     RX2 = (VX2 + VX2T) * DTOC   + RX2T
     RY2 = (VY2 + VY2T.) *DTOC   + RY2T
     INDEX = 0
     GO TO 1005

                                  BLOCK N

1070 P2KE1=0.51804102E-08*(VX1*VX1 + VY1*VY1)*PMASS
     P2KE2= 32.9163268E-08 *(VX2* VX2  +  VY2* VY2)
     TKE = P2KE1 + P2KE2
     WRITE OUTPUT TAPE 3, 15
     WRITE OUTPUT TAPE 3,10
     WRITE OUTPUT TAPE 3, 12, BX, BZ, EV, DTI
     WRITE OUTPUT TAPE 3, 1075
1075 FORMAT(////, 40H RESULTS OF SIMPLE TWO BODY INTERACTION   ,/ )
     WRITE OUTPUT TAPE 3,1080, P2KE1,P2KE2,TKE,EV
10800FORMAT(    15H KIN ENRG PROJ= , F12.5 , 18H    KIN ENRG TARG= ,
    1 F12.5, 14H    TOT ENRG= , F12.5, 12H    ENRG IN= , F10.1, /////)
     WRITE OUTPUT TAPE 3,654
 654 FORMAT(31H RESULTS OF LATTICE INTERACTION ,/, )
     WRITE OUTPUT TAPE 3, 655
655  FORMAT(14H TARGET VALUES ,//,90H  TIME STEPS   PCT E TARGET W/R TO
    1BULLET     KE TARGET     PCT E TARGET W/R TO LAT-BULLET       )
     WRITE OUTPUT TAPE 3,660, CYCLE, POT18 ,PKE8R, PEA8
 660 FORMAT(F10.0,1PE25.6,E18.6,E25.6 )
     WRITE OUTPUT TAPE 3,665,PKE1, COL3, V1X(1),V1Y(1),V1Z(1)
 6650FORMAT(/,14H BULLET VALUES,//,15H   KIN ENERGY = F7.1 , 29H    PCT
    1 E W/R TO LAT-TARGET = F7.1,25H    VELOCITY IN M/SEC  X= 1PE9.2,
    2 4H  Y=  E9.2, 4H  Z=  E9.2  )
     WRITE OUTPUT TAPE 3, 675
 675 FORMAT ( /,  16H LATTICE VALUES    )
     WRITE OUTPUT TAPE 3, 800
 8000FORMAT ( /,     60H     PCT ENERGY     KIN ENERGY    TOT  ENERGY
    1    PER ERROR          )
     WRITE OUTPUT TAPE 3, 810, TPOT , TPKE,  TE, PERE
 810 FORMAT(3F15.5 , F10.5 )
     WRITE OUTPUT TAPE 3, 1100
1100 FORMAT(//, 71H COMPARISON VALUES OF LATTICE REACTION AGAINST SIMPL
    1E TWO BODY PROBLEM ,/, 65H BOTH INTERACTIONS STOPPED WHEN TARGET K
    2INETIC ENERGY MAXIMUM          )
```

```
      T2RA = ATANF(ABSF(VY2/VX2)) *57.296
      B2SA = ATANF(ABSF(VY1/VX1)) * 57.296
      SRE8 = SQRTF(PKE8R/32.9163268E-08)
      SRE1 = SQRTF(PKE1 / (PMASS*0.51804102E-08))
      ATLRA = ABSF(V1Y( 8))/SRE8
      IF(ATLRA-1.0) 1105,1110,1110
 1105 TLRA = ACOSF( ATLRA) * 57.296
      GO TO 1115
 1110 TLRA = 0.0
 1115 ABLSA = ABSF(V1Y( 1))/SRE1
      IF(ABLSA -1.0) 1116,1118,1118
 1116 BLSA = ACOSF( ABLSA) * 57.296
      GO TO 1119
 1118 BLSA = 0.0
 1119 RBMT = PMASS/ 63.54
      ET2 = (P2KE2/EV)*1.0E02
      ETL=(PKE8R/EV)*1.0E02
      RET=ETL/ET2
      RKEP=PKE1/P2KE1
      EABL = TE-PKE1-PKE8R-PPE(8)-PPE(1)
      RSA2L=B2SA/BLSA
      RRA2L = T2RA/TLRA
      RBFI= PKE1/EV
       WRITE OUTPUT TAPE 3,1120,ET2,ETL,RET,RKEP,RBMT
11200FORMAT(/, 43H   PERCENT KE TRANSFERED             TWO BODY=  F9.3,
     118H            LATTICE= F9.3,//, 56H   RATIO KE TRANSFER IN LATTICE
     2/ KE TRANSFER TWO BODY =  F7.5,//,48H   RATIO KE PROJ IN LATTICE /
     3 KE PROJ TWO BODY = F11.5,//, 36H   RATIO BULLET MASS / TARGET MAS
     4S =    F6.3    )
       WRITE OUTPUT TAPE 3,1130,EABL,B2SA,BLSA,T2RA,TLRA,RSA2L,RRA2L
11300FORMAT(/,33H   POT + KE ABSORBED BY LATTICE =   F12.3 ,//,
     1 39H   SCATTERING ANGLE              TWO BODY = F7.2, 19H            LAT
     2TICE =  F7.2,//,35H   RECOIL ANGLE              TWO BODY = F7.2,
     3 19H           LATTICE =  F7.2,//,63H   RATIO SCATTERING ANGLE TWO
     4BODY / SCATTERING ANGLE LATTICE =   F9.5,//,55H   RATIO RECOIL ANG
     5LE TWO BODY / RECOIL ANGLE LATTICE =  F9.5    )
       WRITE OUTPUT TAPE 3,1140, XIP, RBFI
11400FORMAT( /, 21H   IMPACT PARAMETER =  F7.4,  54H      RATIO KE BULLE
     1T AT END OF RUN / ORIGINAL ENERGY =  1PE13.5     )
       WRITE OUTPUT TAPE 3,15
```

```
                                          BLOCK R

      C(1,L) = BX
      C(2,L) = BZ
      C(3,L) = XIP
      IF(BZ-3.0) 1160,1160,1170
 1160 C(4,L) = 0.0
      GO TO 1180
 1170 C(4,L) = ACOSF((BZ-3.0)/XIP)* 57.296
 1180 C(5,L) = ET2*1.0E-02
      C(6,L) = B2SA
      C(7,L) = ETL*1.0E-02
      C(8,L) = BLSA
      C(9,L) = RET
      C(10,L) = PPE(8) + PKE8R
      C(11,L) = TLRA
      C(12,L)=PKE1
      C(13,L)=P2KE1
      C(14,L)= PKE8R
      C(15,L)= P2KE2
      C(16,L)= PERE
      C(17,L)=CYCLE
      C(18,L)= PPE(1)
      C(19,L)= PPE(8)
      C(20,L)= T2RA
      C(21,L)=R1Y(1)
      L=L+1

                                          BLOCK T

      BZ= BZ-0.1
      IF(BZS-BZ)5,5,1300
 1300 CONTINUE
      IF(SENSE SWITCH 1) 3, 4000
 4000 CONTINUE
```

BLOCK W

```
      LMAX = L-1
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1350
 1350 FORMAT(//,110H         X          Z          B            ANGLE     TM(2)
     1SANGLE     TM(L)     SANGLE   TM(L)/TM(2)    TE TAR     RANGLE      ,/ )
      DO 1360 J=1,LMAX
 1360 WRITE OUTPUT TAPE 3,1400,(C(I,J), I= 1,11  )
 1400 FORMAT(3F9.3,F10.2,F10.4,F10.2,F10.4,F10.2,F10.4,F13.4,F10.2)
      DO 1500  M= 1,5
      WRITE OUTPUT TAPE 3,15
      J = 12
      I = 14
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1450
 1450 FORMAT(//,33X53H TOP NO. IS KINETIC ENERGY IN EV OF BULLET IN LATT
     1ICE,//,32X57H BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN LATT
     2ICE     )
 1500 WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
      DO 1530   M = 1,5
      WRITE OUTPUT TAPE 3,15
      J=12
      I=13
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1510
 1510 FORMAT(//, 33X53H TOP NO. IS KINETIC ENERGY IN EV OF BULLET IN LAT
     1TICE,//,28X64H BOTTOM NO. IS KINETIC ENERGY IN EV OF BULLET IN TWO
     2BODY PROBLEM   )
 1530 WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
      DO 1550 M= 1,5
      WRITE OUTPUT TAPE 3,15
      J = 14
      I = 15
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1540
 1540 FORMAT(//, 33X53H TOP NO. IS KINETIC ENERGY IN EV OF TARGET IN LAT
     1TICE,//, 27X66H BOTTOM NO. IS KINETIC ENERGY IN EV OF TARGET IN TW
     2O BODY PROBLEM  )
 1550 WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
      WRITE OUTPUT TAPE 3,15
      J=17
      I=16
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1560
 1560 FORMAT(//, 44X32H TOP NO. IS NUMBER OF TIME STEPS,//,46X28H BOTTOM
     1 NO. IS PERCENT ERROR  )
      WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
```

```
      DO 1580  M=1,2
      WRITE OUTPUT TAPE 3,15
      J=8
      I=6
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1570
 1570 FORMAT(//, 40X39H TOP NO. IS SCATTERING ANGLE IN LATTICE,//,34X52H
     1 BOTTOM NO. IS SCATTERING ANGLE OF TWO BODY PROBLEM   )
 1580 WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
      DO 1600  M=1,2
      WRITE OUTPUT TAPE 3,15
      J=11
      I=20
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1590
 1590 FORMAT(//, 42X35H TOP NO. IS RECOIL ANGLE IN LATTICE,//,36X47H BOT
     1TOM NO. IS RECOIL ANGLE OF TWO BODY PROBLEM   )
 1600 WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
      DO 1620  M=1,5
      WRITE OUTPUT TAPE 3,15
      J=19
      I=18
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1610
 1610 FORMAT(//,32X55H TOP NO. IS POTENTIAL ENERGY IN EV OF TARGET IN LA
     1TTICE,//, 31X58H BOTTOM NO. IS POTENTIAL ENERGY IN EV OF BULLET IN
     2 LATTICE    )
 1620 WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
      DO 1640 M=1,2
      WRITE OUTPUT TAPE 3,15
      J=21
      I=12
      WRITE OUTPUT TAPE 3,1425
      WRITE OUTPUT TAPE 3,10
      WRITE OUTPUT TAPE 3,1430,EV,DTI
      WRITE OUTPUT TAPE 3,1630
 1630 FORMAT(//,36X47H TOP NO. IS BULLET PENETRATION IN LATTICE UNITS,//
     1,32X56H BOTTOM NO. IS KINETIC ENERGY IN EV OF BULLET IN LATTICE   )
 1640 WRITE OUTPUT TAPE 3,1850,(C(J,L), L=1,11), (C(I,L), L=1,11),
     1(C(J,L), L=12,20), (C(I,L), L=12,20), (C(J,L), L=21,27),
     2(C(I,L), L=21,27), (C(J,L), L=28,32), (C(I,L), L=28,32),
     3(C(J,L), L=33,35), (C(I,L), L=33,35), C(J,36),C(I,36)
 1425 FORMAT(/////////)
 1430 FORMAT(/, 8X25H BULLET INCOMING ENERGY = ,F8.1,31H  EV      TIME ST
     1EP MULTIPLIER = ,F5.3, 34H      BULLET INCIDENT ON (100) FACE   )
 1850 FORMAT(////,3X11F10.3,/,111H        *         *         *
     1 *         *         *         *         *         *         *
     2     * ,/,3X11F10.3,//////,13X9F10.3,/, 18X82H *         *
     3 *         *         *         *         *         *         * ,/,
     413X9F10.3,//////,23X7F10.3,/,28X62H *         *         *
     5*         *         *         *,/,23X7F10.3,//////,33X5F10.3,/,38X
     642H *         *         *         *         *,/,33X5F10.3,//////,4
     73X3F10.3,/,48X22H *         *        *,/,43X3F10.3,//////,53XF10.
     83,/,58X2H *,/,53XF10.3)
      END
```

BLOCK Y

```
FUNCTION POTF(DIST)
COMMON ETFP,AFAC,ETFF
POTF=ETFP*(1.0+(DIST*AFAC)**0.8034)**(-3.734)/DIST
RETURN
END
```

BLOCK Z

```
FUNCTION FORC(DIST)
COMMON ETFP,AFAC,ETFF
Y=(DIST*AFAC)**0.8034
YP=1.0+Y
Z=YP**(-3.734)
FORC=ETFF*Z*(1.0+2.9999*Y/YP)/(DIST*DIST)
RETURN
END
END
```

APPENDIX VI

POTENTIALS

1. Born-Mayer

A. Potential

$$\phi(r) = Ae^{-\rho(r-r_o)/r_o}$$

r_o = nearest neighbor separation at zero pressure and absolute zero

r_o for copper = 2.51A

The three different sets of constants used in the potential form are identical to those used by Gibson et. al.[16]

Potential	A(ev)	ρ
1	0.0392	16.97
2	0.051	13.00
3	0.1004	10.34

Potential No. 2 was used extensively in the program. It can be reduced to a simplified form in the following manner:

$$\phi(r) = 0.051 \times e^{-13.0(r-2.551)/2.551}$$

if distances are expressed in lattice units

$$\phi(r) = 0.051 \times e^{(13.0-9.208\,r)}$$

in the potential function subroutine this becomes

```
POTF = 0.051 * EXPF(13.0-DIST * 9.208)
```

Potentials one and three become;

```
1)  POTF = 0.0392 * EXPF(16.97-DIST * 8.9996)

3)  POTF = 0.1004 * EXPF(10.34-DIST * 7.3115)
```

B. Force

$$\frac{\partial[\phi(r)]}{\partial r} = -Ae^{-\rho(r-r_0)/r_0} \times \frac{\rho}{r_0}$$

substitution of constants for Potential No. 2

$$\frac{\partial[\phi(r)]}{\partial r} = -\frac{(13.0)(0.051)}{2.551}\, e^{-13.0(r-2.551)/2.551}$$

if distances are expressed in lattice units and electron volts changed to joules;

$$\frac{\partial[\phi(r)]}{\partial r} = -0.41614 \times 10^{-9} \times e^{(13.0-9.208r)}$$

in the force function subroutine this becomes;

```
FORC = 0.41614E-09 * EXPF(13.0-9.208*DIST)
```

forces for potentials one and three become;

```
1) FORC = 0.3127E-09*EXPF(16.97-8.9996*DIST)
2) FORC = 0.6507E-09*EXPF(10.34-7.3115*DIST)
```

2. Thomas-Fermi-Firsov

A. Potential

$$V(r) = \frac{1}{2} E_{TF} \left[\left(\frac{a_{TF}}{r}\right) \phi\left(\frac{r}{a_{TF}}\right) \right]$$

$$\phi\left(\frac{r}{a_{TF}}\right) = \phi(x)$$ Thomas-Fermi screening function

$$\phi(x) = \left[1 + \left(\frac{x}{\alpha_1}\right)^{\alpha_2} \right]^{-\alpha_3}$$

$$\alpha_1 = 12^{2/3} \qquad E_{TF} = 2 Z_1 Z_2 e^2 / a_{TF}$$

$$\alpha_2 = 0.8034$$

$$\alpha_3 = 3.734 \qquad a_{TF} = \frac{\left(9\pi^2/128\right)^{\frac{1}{3}} k\, a_H}{\left(\sqrt{Z_1} + \sqrt{Z_2}\right)^{2/3}}$$

$a_H = \hbar^2 / me^2$ first Bohr radius of hydrogen

$$K = 1 \qquad E_{TF} = 219233 \text{ ev} \qquad a_{TF} = .96062 \times 10^{-11} \text{ m}$$

let $x = r/a_{TF}$ and ATFR = $1/a_{TF}$ (in lattice units)

then x = ATFR * DIST (DIST in lattice units)

$$\phi(x) = \left[1 + \left(\frac{x}{\alpha_1}\right)^{\alpha_2}\right]^{-\alpha_3} = \left[1 + \left(\frac{\text{ATFR} \times \text{DIST}}{\alpha_1}\right)^{\alpha_2}\right]^{-\alpha_3}$$

let ATFR/α_1 = AFAC

$$\phi(x) = \left[1 + (\text{AFAC} \times \text{DIST})^{0.8034}\right]^{-3.734}$$

$$V(r) = \left[\frac{E_{TF}}{2}\right] \frac{1}{x} \phi(x) = \frac{E_{TF} \times \phi(x)}{2 \times \text{ATFR} \times \text{DIST}}$$

let ETFP = E_{TF}/ 2 * ATFR

then

$$\text{POTF} = \frac{\text{ETFP}}{\text{DIST}} \left[1.0 + (\text{AFAC} * \text{DIST})^{0.8034}\right]^{-3.734}$$

B. Force

set $x = r/a_{TF}$

$$\frac{\partial(V(r))}{\partial r} = \frac{\partial(V(r))}{\partial x} \times \frac{\partial x}{\partial r}$$

$$\frac{\partial(V(r))}{\partial r} = \frac{E_{TF}}{2}\left[-\frac{\phi(x)}{x^2} + \frac{1}{x}\frac{d(\phi(x))}{dx}\right] \times \frac{1}{a_{TF}}$$

set $Y = (x/\alpha_1)^{\alpha_2}$

then

$$\frac{d(\phi(x))}{dx} = -\alpha_2\alpha_3 \frac{\phi(x)}{x}\frac{Y}{1+Y}$$

$$\frac{\partial(V(r))}{\partial r} = \frac{E_{TF} \times a_{TF}}{2r^2}\left[1 + \alpha_2\alpha_3\frac{Y}{Y+1}\right] \times \phi(x)$$

if the following substitutions and appropriate changes in units are made

$$FORC = \frac{ETFF * Z}{DIST * DIST}\left[1.0 + 2.9999 * \frac{Y}{YP}\right]$$

where $ETFF = E_{TF} * a_{TF} /2$

x = DIST * AFAC (DIST in lattice units)

$$Y = (x)^{0.8034} \qquad YP = 1.0 + Y$$

$$Z = (YP)^{-3.734}$$

ETFF and AFAC are defined at the beginning of the program - Y, YP and Z are calculated in the subroutine each time it is used.

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